



UNIVERSITÉ
CÔTE D'AZUR



Stretching in isotropic turbulence: Polymers and elastic filaments

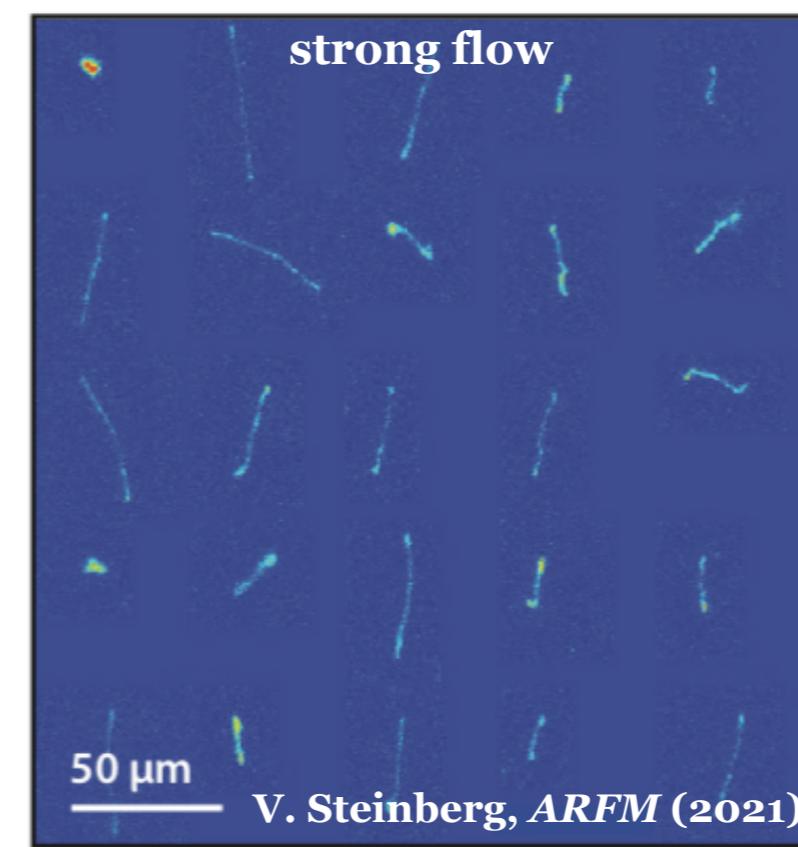
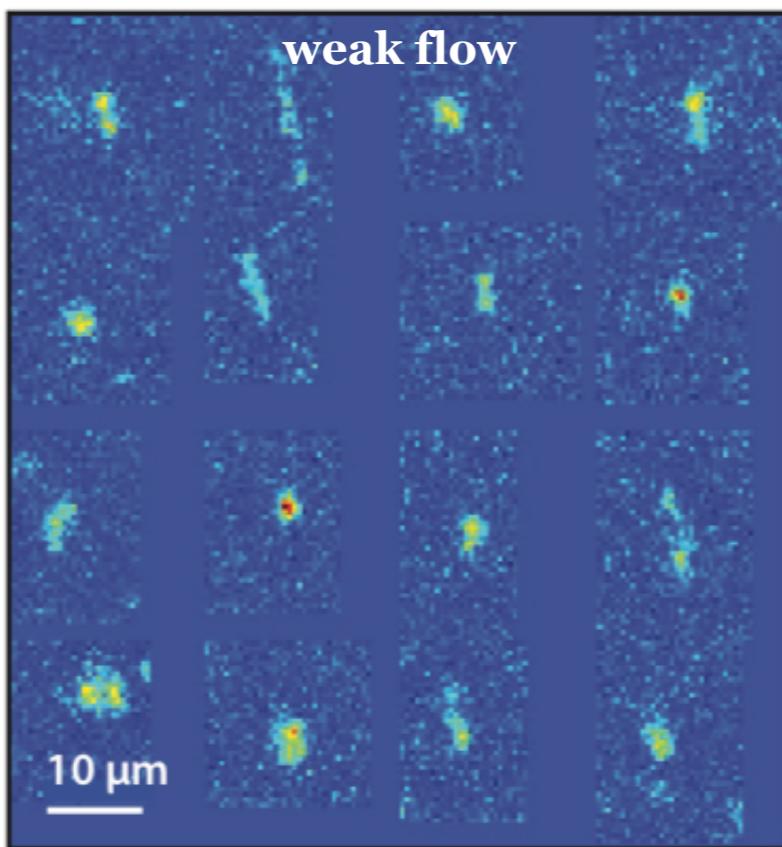
Dario Vincenzi

Université Côte d'Azur, CNRS, Laboratoire J.A. Dieudonné, Nice, France

Outline

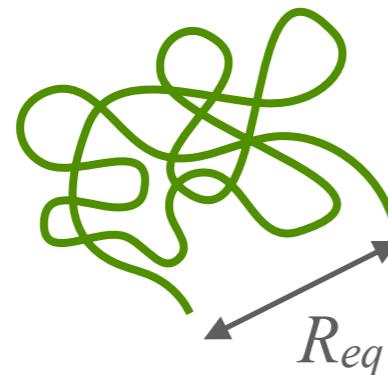
- Polymer modelling
- Coil-stretch transition in extensional flows
- Random and turbulent flows
 - ♦ PDF of the extension
 - * Large deviations theory
 - * Batchelor–Kraichnan model
 - * Lagrangian simulations
 - * Micro-fluidics experiments
 - ♦ Relaxation to steady state
 - ♦ Breakup
 - ♦ Stretching beyond the Kolmogorov scale
- Elastic filaments
- Perspectives

Polymer dynamics in a flow field



Polymers in a flow field: dimensionless parameters

Extensibility parameter $b = (L / R_{eq})^2$



equilibrium end-to-end separation

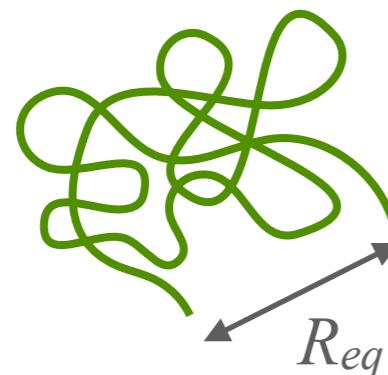


contour length

In experiments: polystyrene, PEO, PAM, and DNA; $10's \mu\text{m} \lesssim L \lesssim 1\text{mm}$, $10^2 \lesssim b \lesssim 10^4$

Polymers in a flow field: dimensionless parameters

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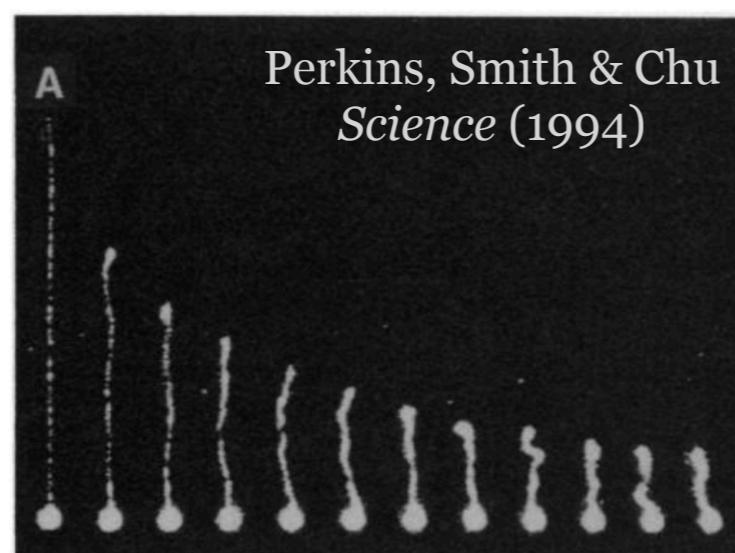
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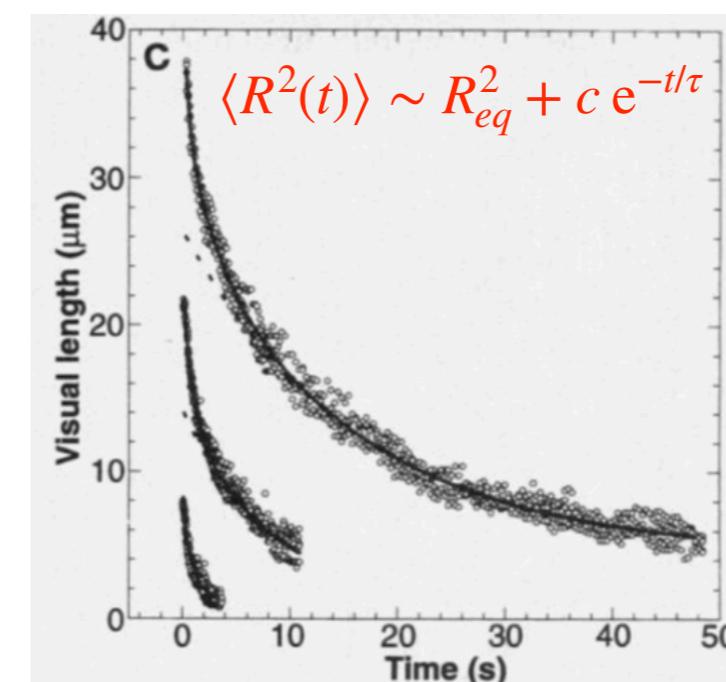
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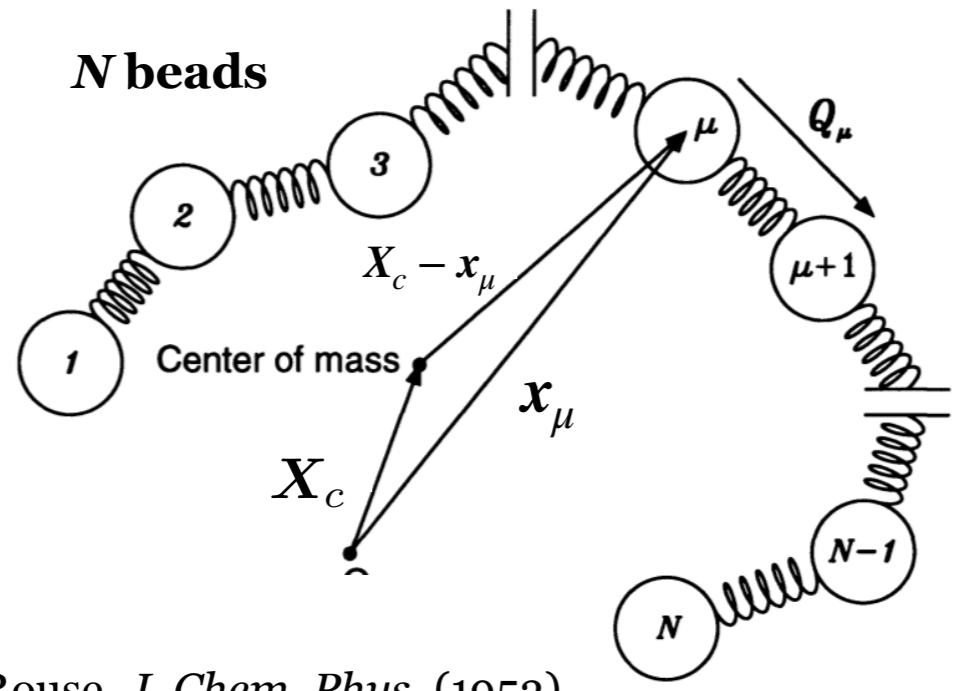
Weissenberg number $\text{Wi} = \tau / T_{\text{flow}}$



DNA with $L \approx 40\mu\text{m}$, sucrose or glycerol solution

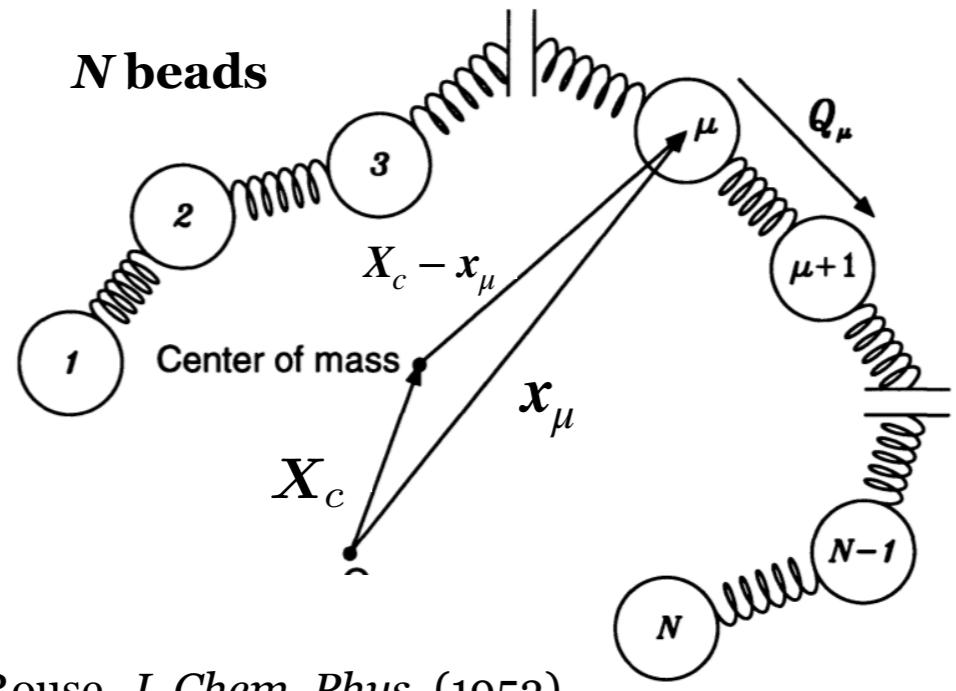


Polymer models: The bead–spring chain



Rouse, *J. Chem. Phys.* (1953)

Polymer models: The bead–spring chain

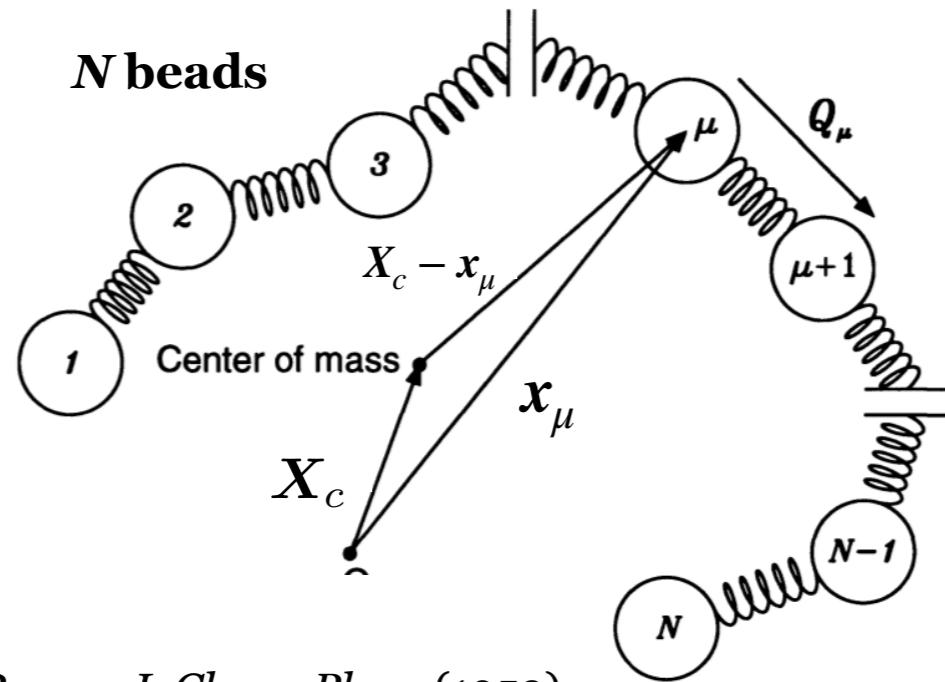


Rouse, *J. Chem. Phys.* (1953)

Forces on the i -th bead

1. Stokes drag: $F_i^d = -\zeta[\dot{x}_i - \mathbf{u}(\mathbf{x}_i, t)]$
2. Thermal noise: $F_i^B = \sqrt{2K_B T / \zeta} \xi_i(t)$ with $\xi_i(t)$ independent white noises
3. Elastic force: $F_i^{\text{el}} = k f_i (\mathbf{x}_{i+1} - \mathbf{x}_i) + k f_{i-1} (\mathbf{x}_{i-1} - \mathbf{x}_i)$

Polymer models: The bead–spring chain



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Elastic coefficient

$$f_i = 1 \quad (\text{Hooke})$$

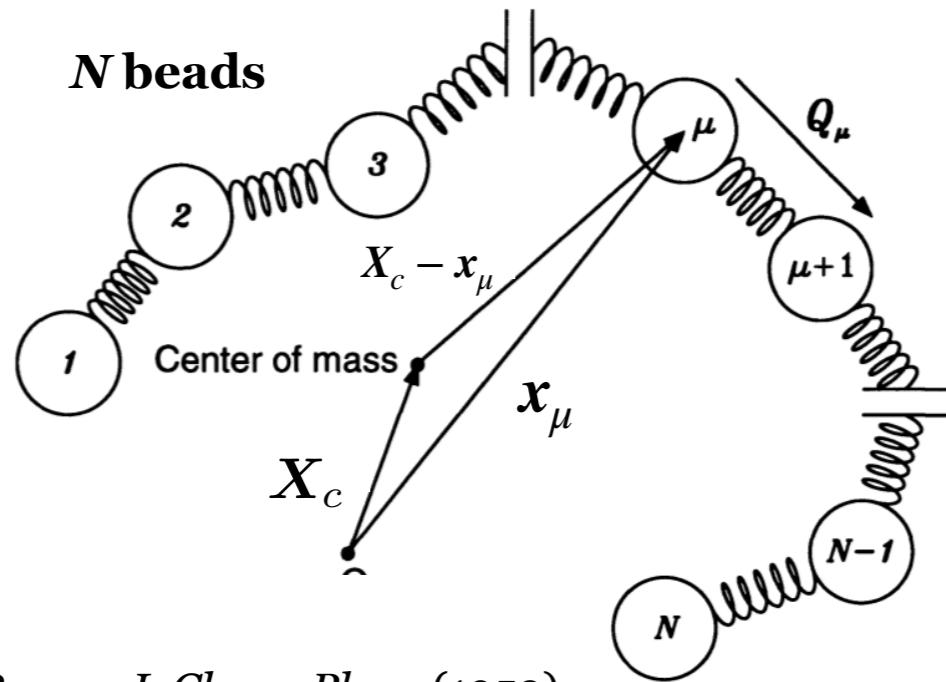
$$f_i = \frac{1}{1 - Q_i^2/\ell^2}, \quad Q_i = |x_{i+1} - x_i| \quad (\text{FENE})$$

$$f_i = \frac{2}{3} - \frac{\ell}{6Q_i} + \frac{\ell}{6Q_i(1 - Q_i/\ell)^2} \quad (\text{Marko-Siggia})$$

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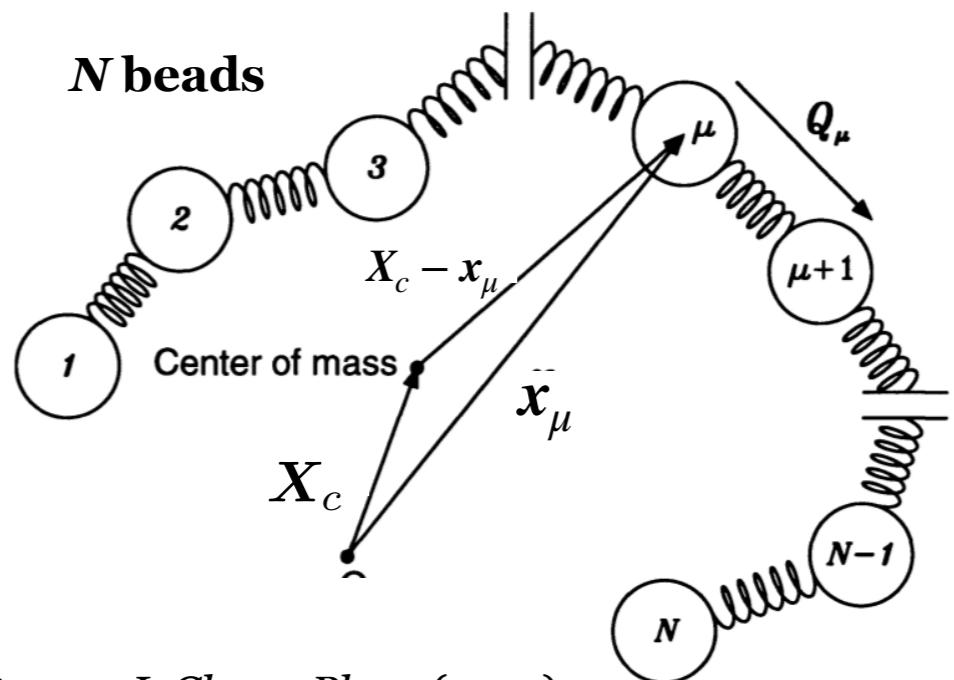
Assumptions

Negligible *hydrodynamic* and *excluded-volume* interactions

Negligible inertia: $m\ddot{x}_i = 0$ and hence $\mathbf{F}_i^d + \mathbf{F}_i^{\text{el}} + \mathbf{F}_i^B = 0$

Linear velocity field: $\mathbf{u}(x_{i+1}) - \mathbf{u}(x_i) = \nabla \mathbf{u} \cdot (x_{i+1} - x_i)$

Polymer models: The bead–spring chain

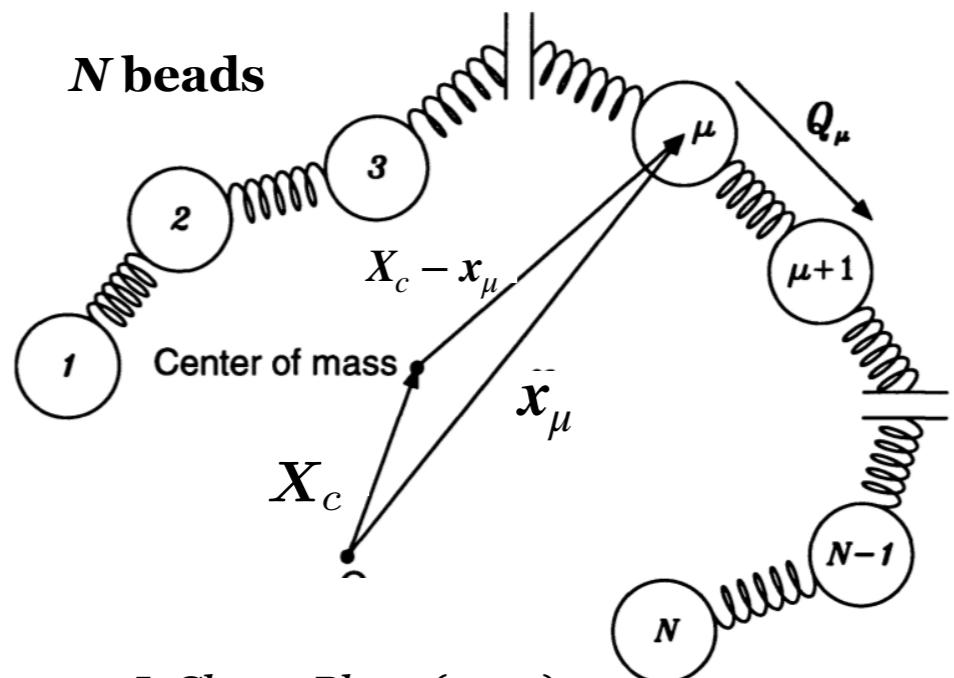


Rouse, *J. Chem. Phys.* (1953)

$$\frac{dX_c}{dt} = \mathbf{u}(X_c, t) + \frac{1}{N} \sqrt{\frac{R_{eq}^2}{6\tau}} \sum_{i=1}^N \xi_i(t)$$

$$\frac{dQ_i}{dt} = \nabla \mathbf{u} \cdot \mathbf{Q}_i - \frac{1}{4\tau} (2f_i \mathbf{Q}_i - f_{i+1} \mathbf{Q}_{i+1} - f_{i-1} \mathbf{Q}_{i-1}) + \sqrt{\frac{R_{eq}^2}{6\tau}} [\xi_{i+1}(t) - \xi_i(t)], \quad \tau = 4k/\zeta$$

Polymer models: The bead–spring chain



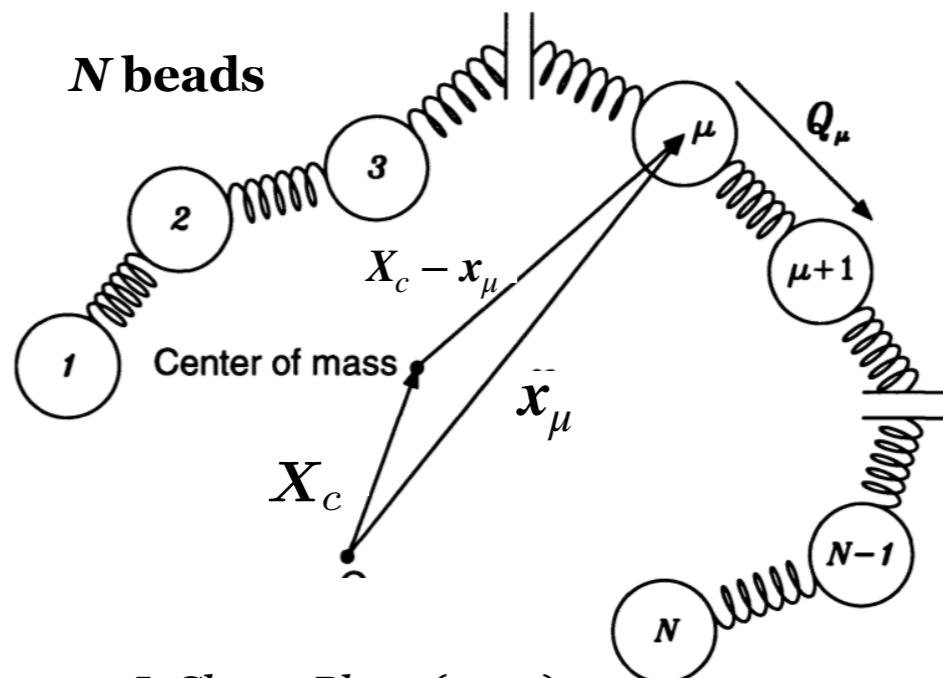
Rouse, *J. Chem. Phys.* (1953)

$$\tau_{\text{chain}} = \frac{6\tau}{N(N+1)}$$
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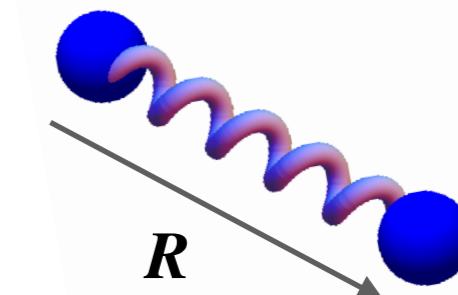
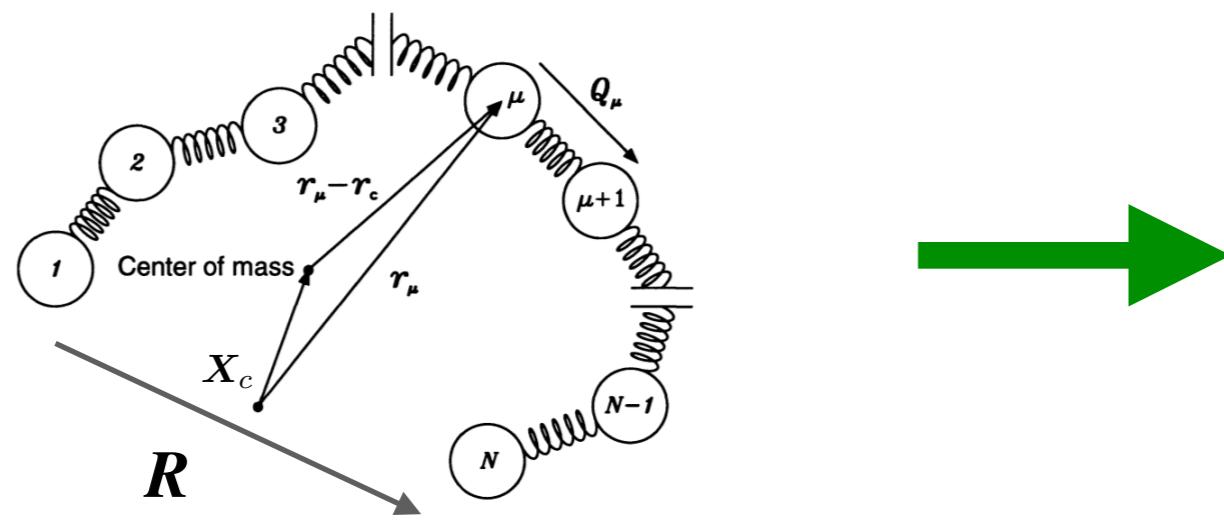
Doi & Edwards, *The Theory of Polymer Dynamics* (Oxford University Press, 1986)

Bird, Curtiss, Armstrong & Hassager, *Dynamics of Polymeric Liquids*, Vol. 2 (Wiley, 1987)

Öttinger, *Stochastic Processes in Polymeric Fluids* (Springer, 1996)

Graham, *Microhydrodynamics, Brownian Motion, and Complex Fluids* (Cambridge University Press, 2018)

Polymer models: The dumbbell model ($N = 2$)



$$\frac{d\mathbf{R}}{dt} = \nabla u \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{\text{eq}}^2}{3\tau}} \xi(t)$$

Associated Fokker–Planck equation for the PDF of \mathbf{R} : $\psi(\mathbf{R}, t)$

$$\frac{\partial \psi}{\partial t} = - \frac{\partial}{\partial R_i} \left\{ \left[\partial_j u_i R_j - \frac{f(R)}{2\tau} R_i \right] \psi \right\} + \frac{R_{\text{eq}}^2}{6\tau} \frac{\partial^2 \psi}{\partial R_i \partial R_i}$$

Continuum models of polymer solutions (Oldroyd-B, FENE-P, ...)

Polymer conformation tensor $\mathbf{C} = \langle \mathbf{R} \otimes \mathbf{R} \rangle_\xi$

Coil-stretch transition in an extensional flow

P.-G. De Gennes, *J. Chem. Phys.* (1974); E.J. Hinch, *Colloques Internationaux du CNRS* (1975)

2D extensional flow

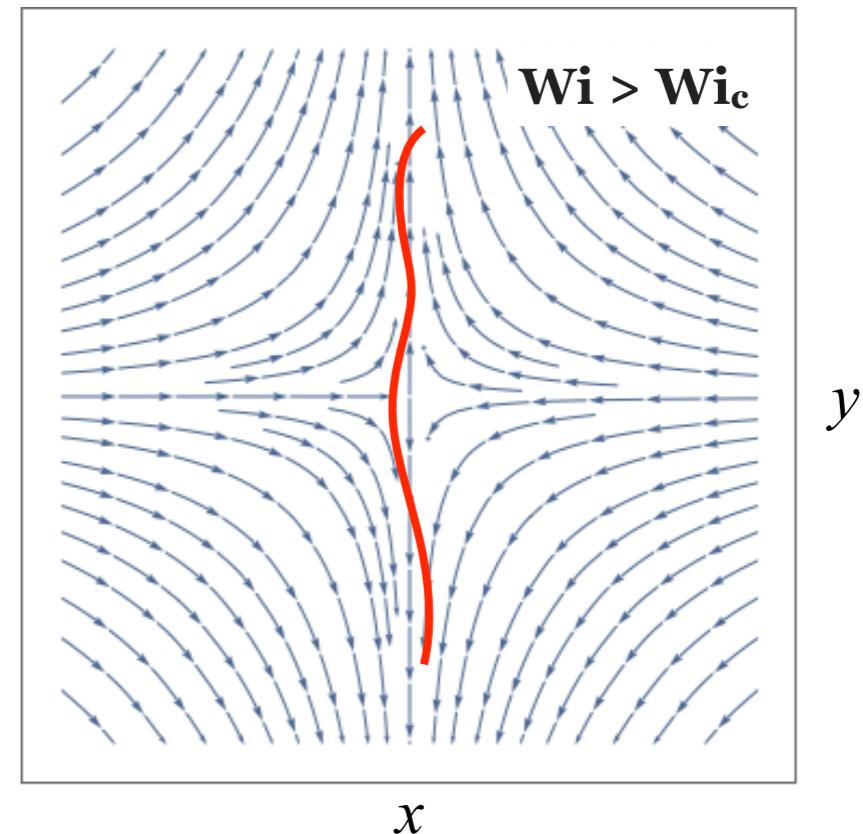
$$\mathbf{u} = \gamma(-x, y), \quad \text{Wi} = \gamma\tau$$

$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{\text{eq}}^2}{3\tau}} \xi(t)$$

Neglect the noise and consider linear elasticity:

$$\dot{R}_x = - \left(\gamma + \frac{1}{2\tau} \right) R_x$$

$$\dot{R}_y = - \left(\gamma - \frac{1}{2\tau} \right) R_y$$



$$R \sim R_y \sim R_0 e^{(\text{Wi} - \text{Wi}_{\text{crit}}) t/\tau}, \quad \text{Wi}_{\text{crit}} = 1/2$$

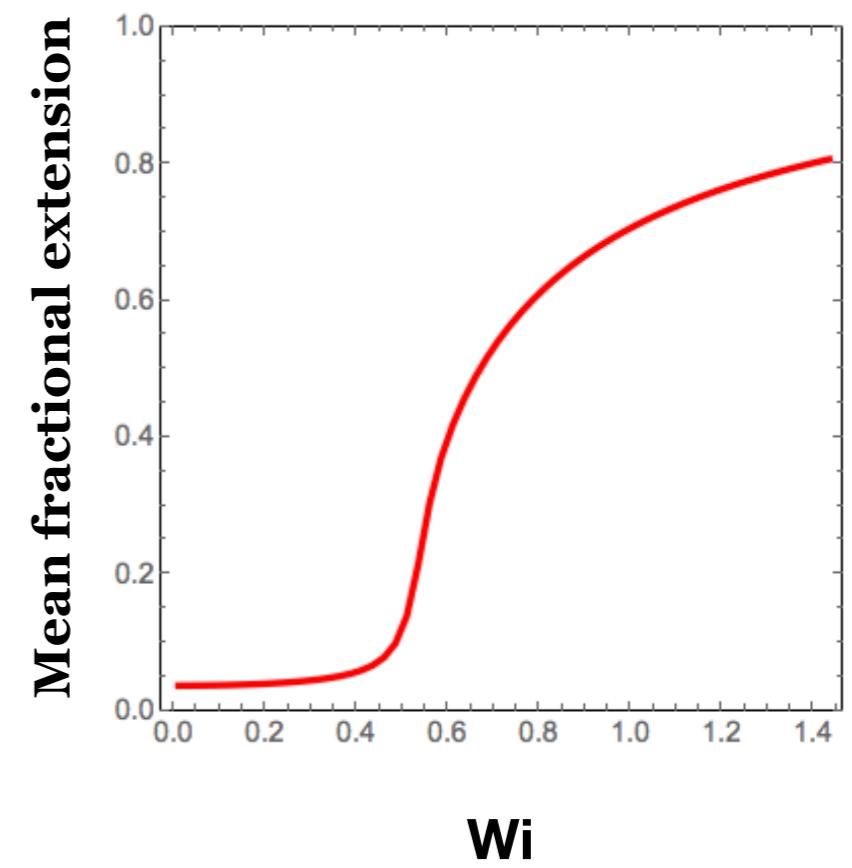
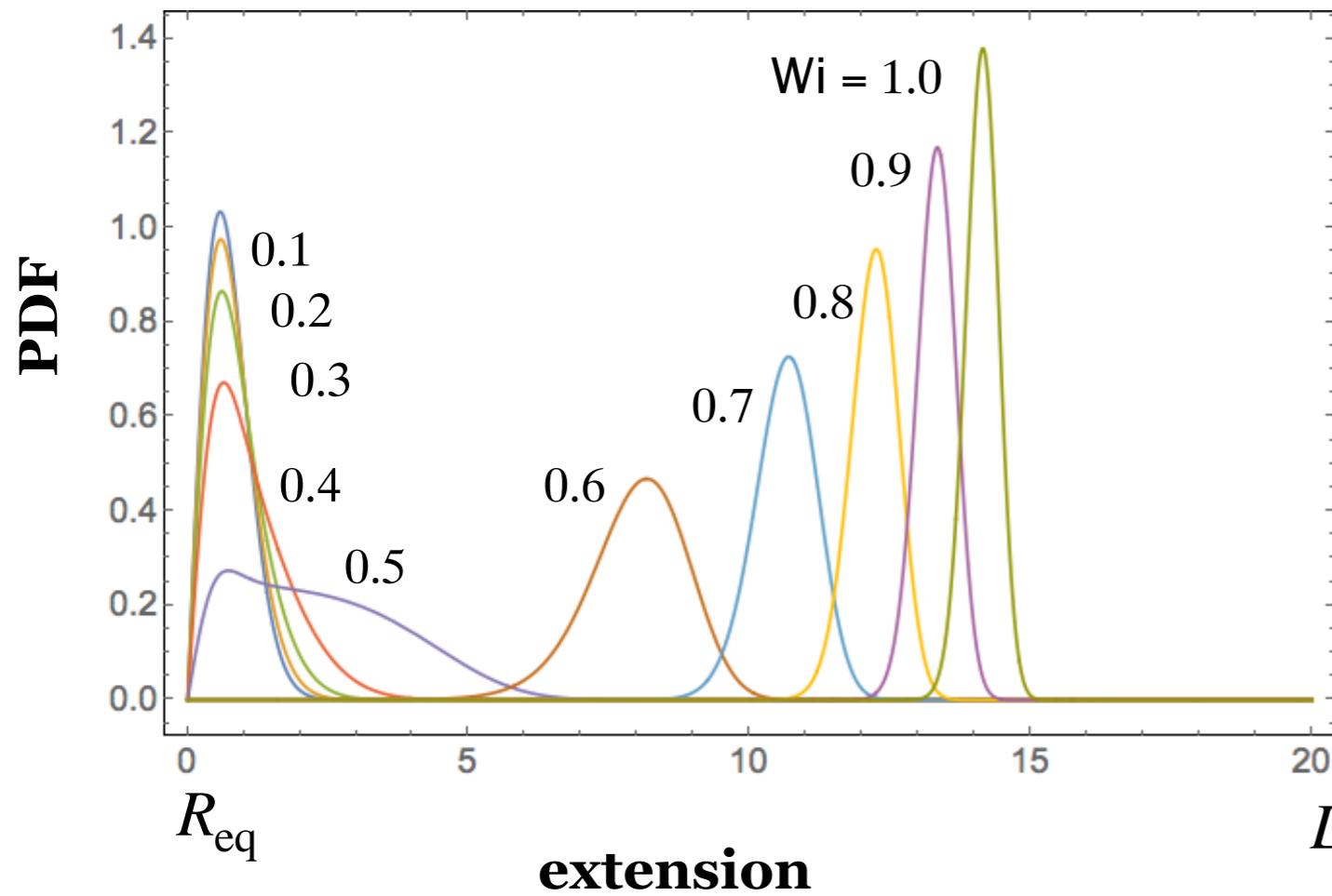
Coil-stretch transition in an extensional flow

FENE model (nonlinear elasticity)

$$F^{\text{el}} = \frac{R}{1 - R^2/L^2}$$

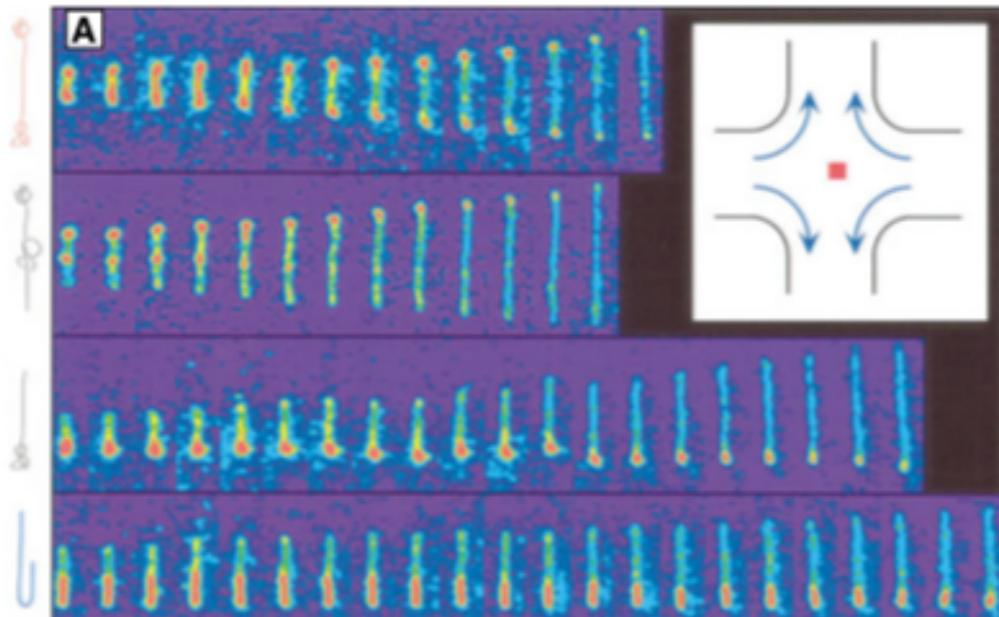
If \mathbf{u} is steady, potential, and $\nabla \mathbf{u} = (\nabla \mathbf{u})^\top$:

$$\psi_{\text{st}}(\mathbf{R}) \propto e^{-3\Phi/R_{\text{eq}}^2} e^{3\tau R_{\text{eq}}^{-2}(\nabla \mathbf{u} : \mathbf{R}\mathbf{R})} \quad \text{with} \quad F^{\text{el}} = -\nabla \Phi$$

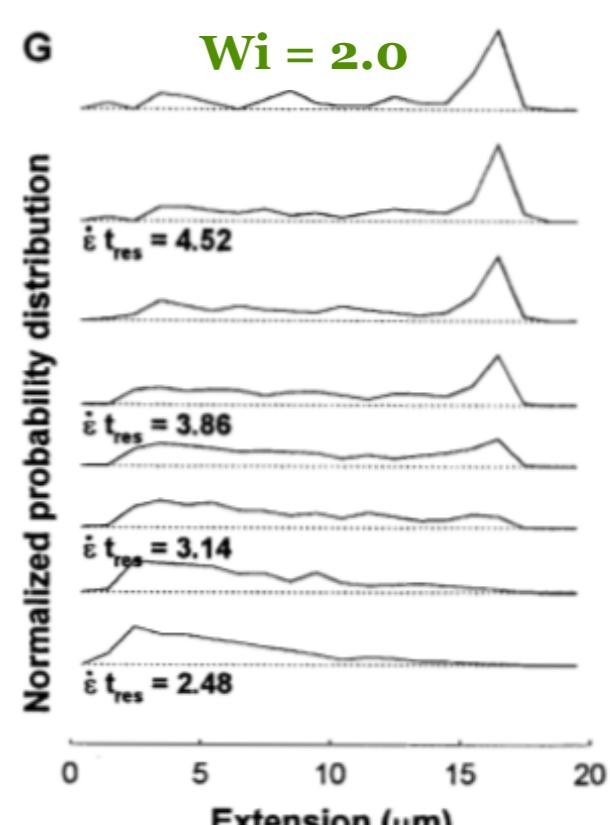
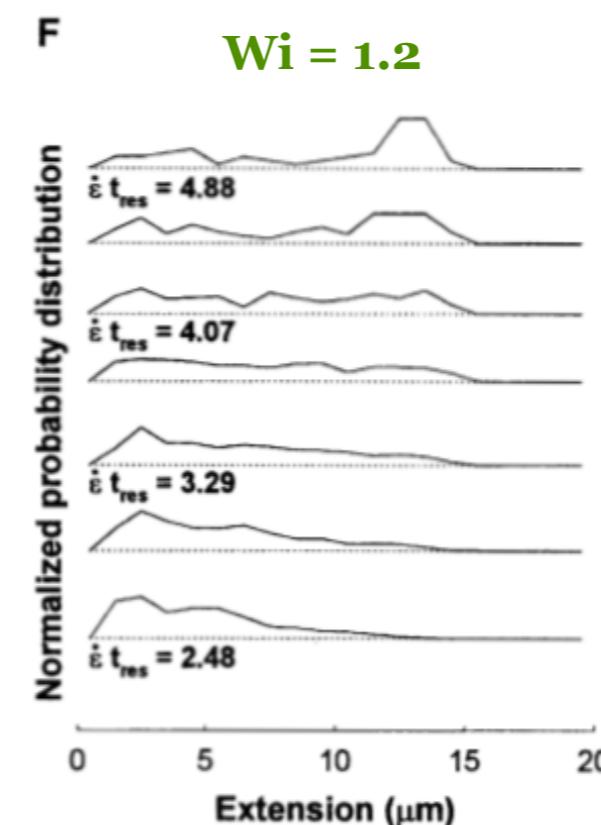
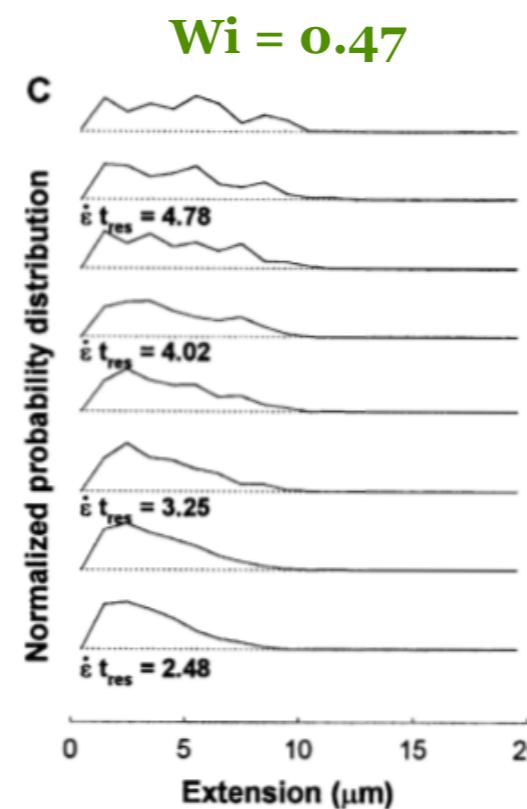
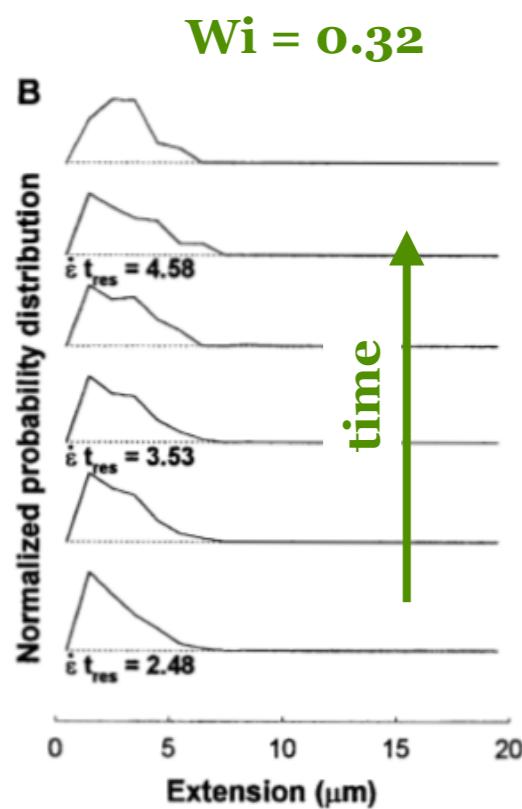
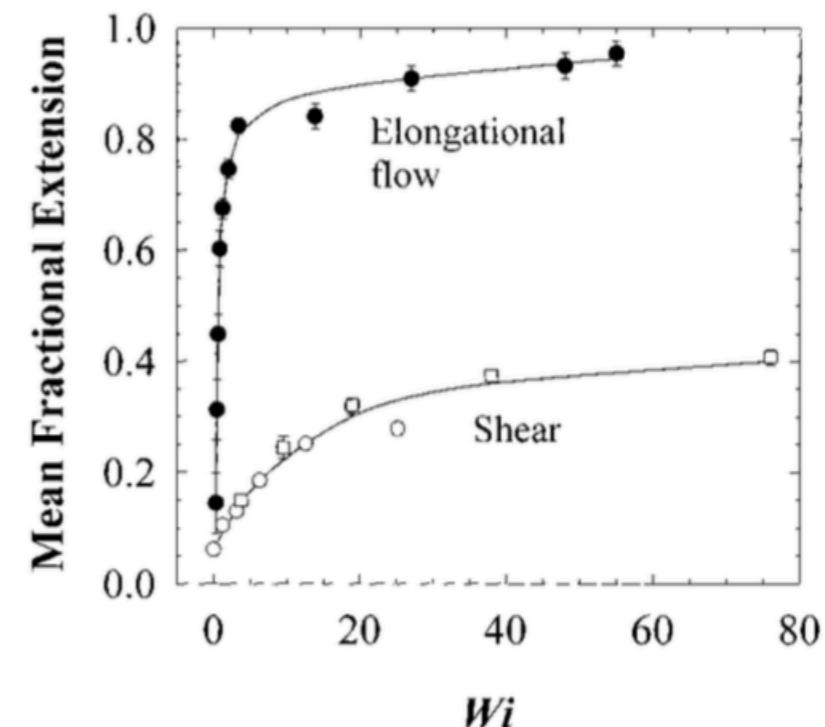


Coil-stretch transition in an extensional flow

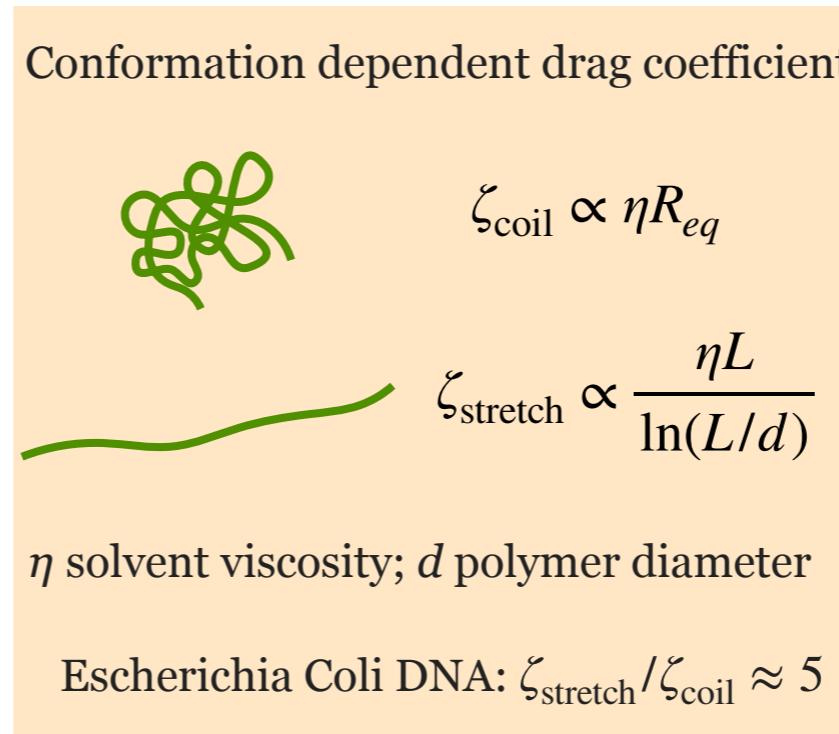
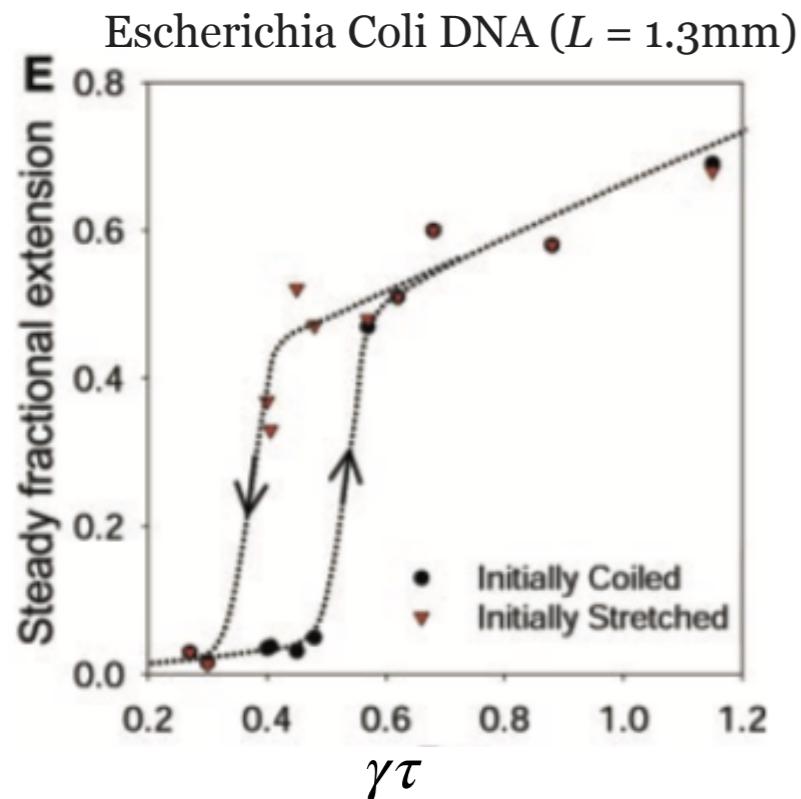
Perkins, Smith & Chu, *Science* (1997)



Smith, Babcock & Chu, *Science* (1999)

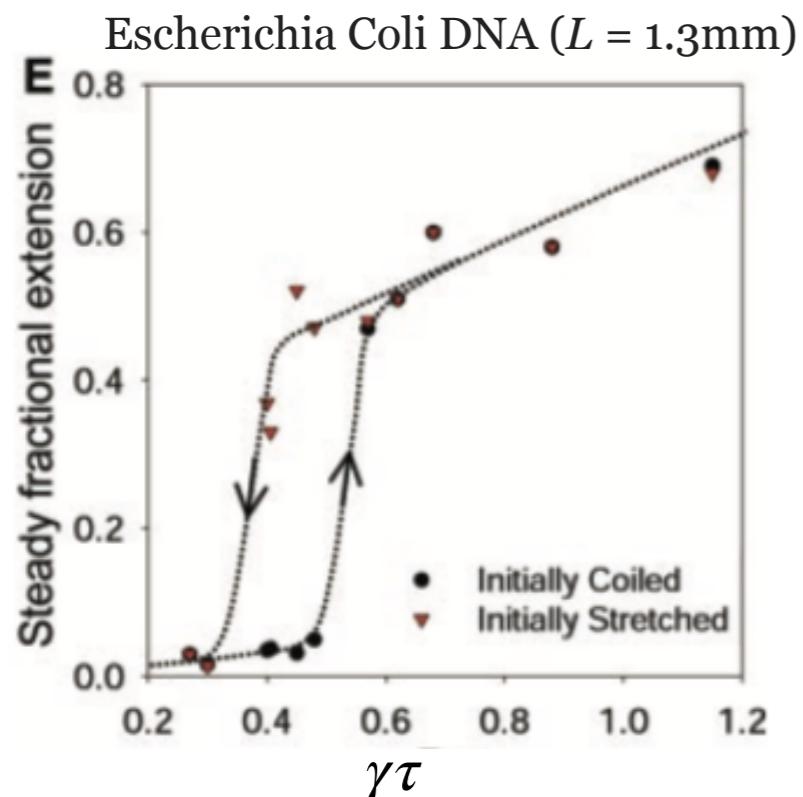


Hysteresis

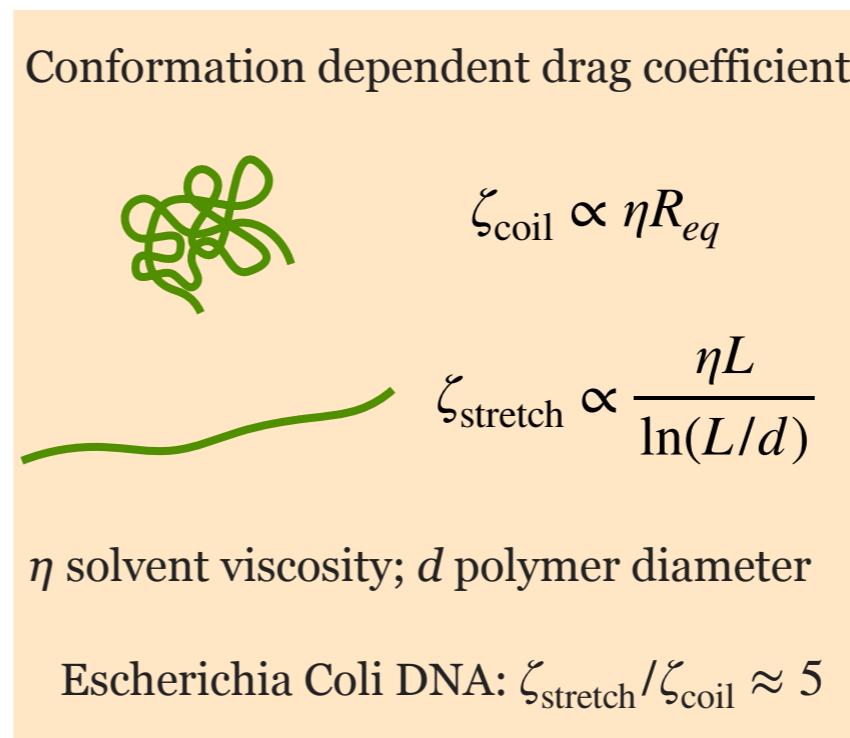


Schroeder, Babcock, Shaqfeh & Chu, *Science* (2003)

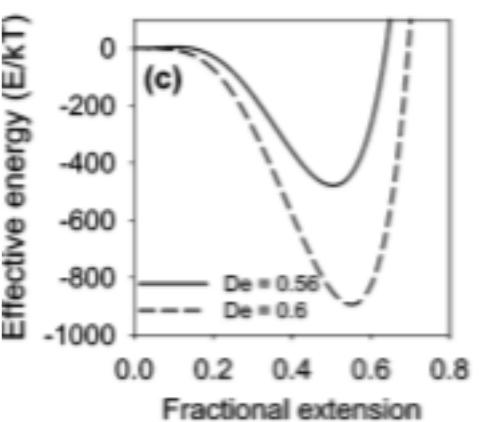
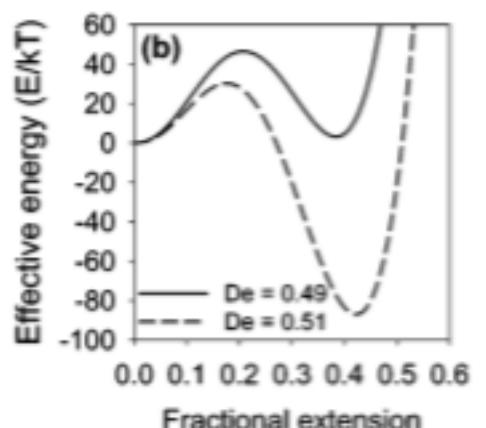
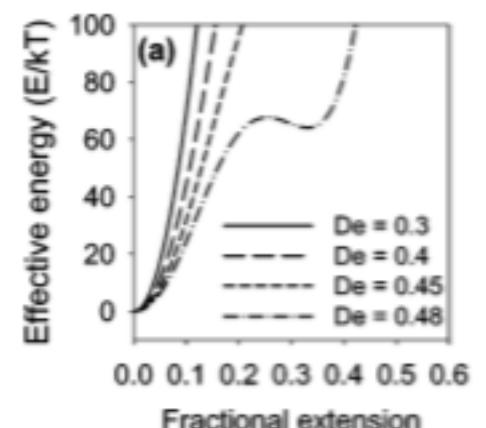
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Schroeder, Babcock, Shaqfeh & Chu, *Science* (2003)

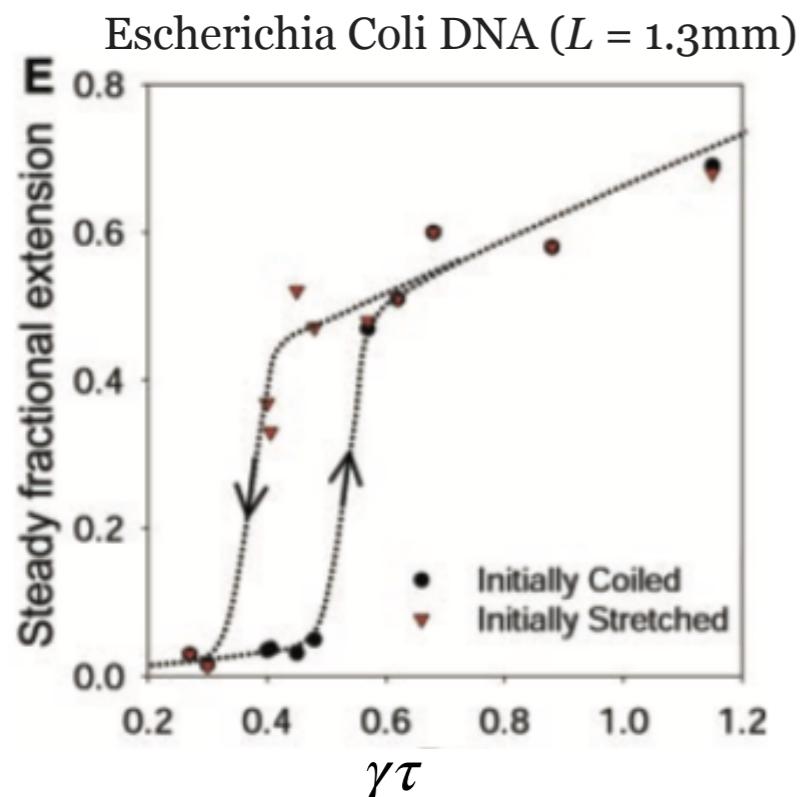


$$\psi_{\text{st}}(R) \propto e^{-E(R)/K_B T}$$

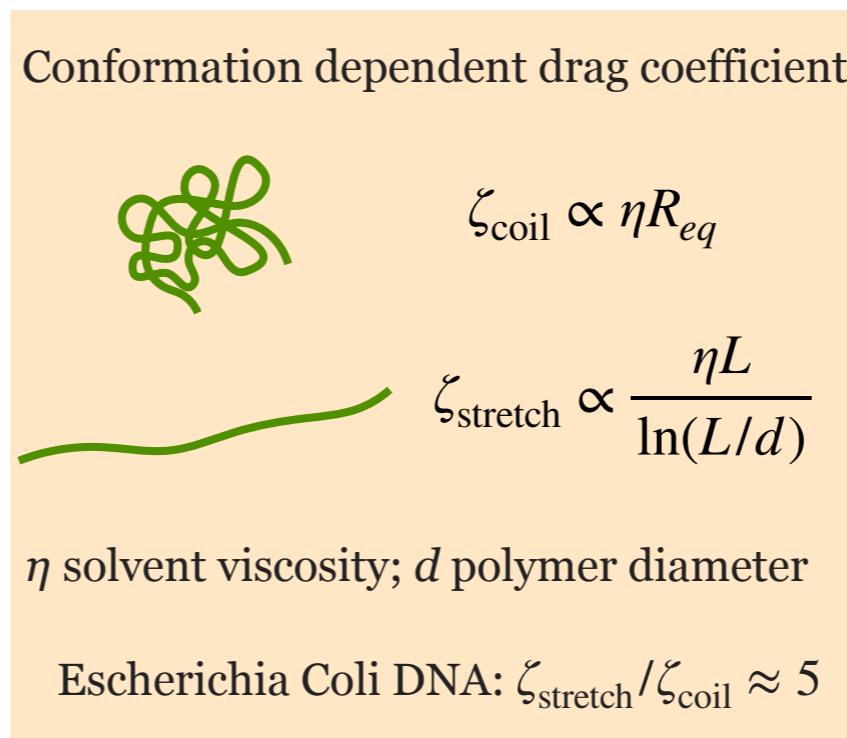


Schroeder, Shaqfeh & Chu
Macromolecules (2004)

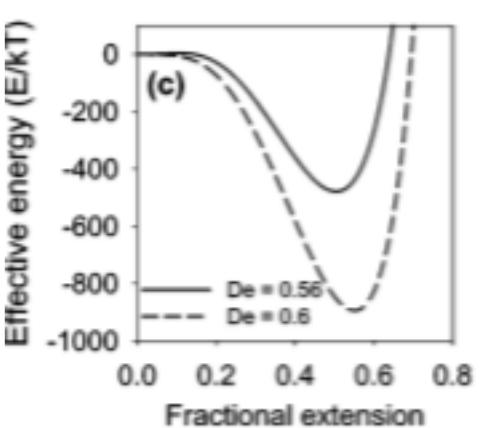
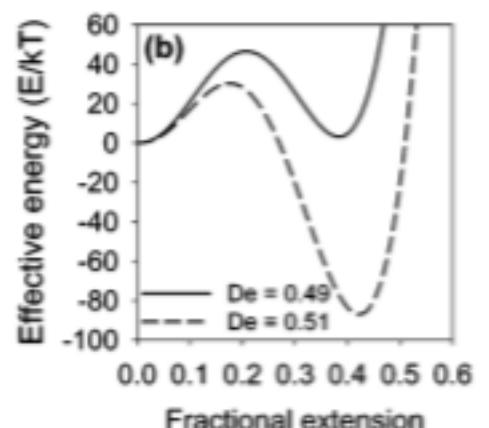
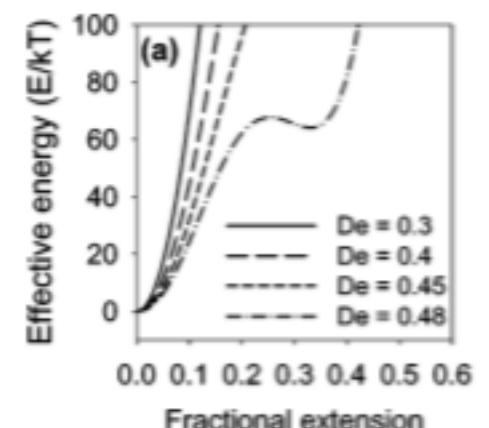
Hysteresis



Schroeder, Babcock, Shaqfeh & Chu, *Science* (2003)



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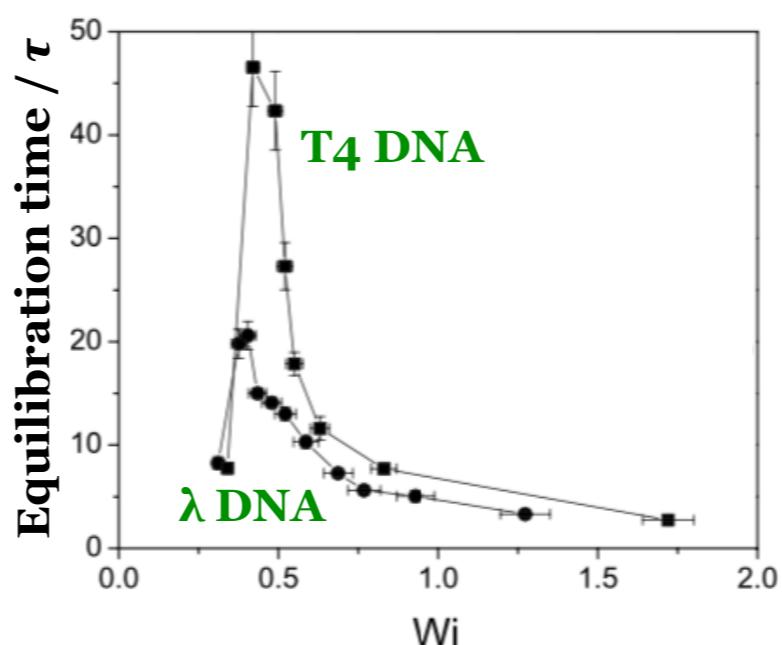


Critical slowing down

Gerashchenko & Steinberg,
Phys. Rev. E (2008)

■ T4 DNA, $L = 67\mu\text{m}$,
 $\zeta_s/\zeta_c = 2.1$

● λ DNA, $L = 21\mu\text{m}$,
 $\zeta_s/\zeta_c = 1.6$



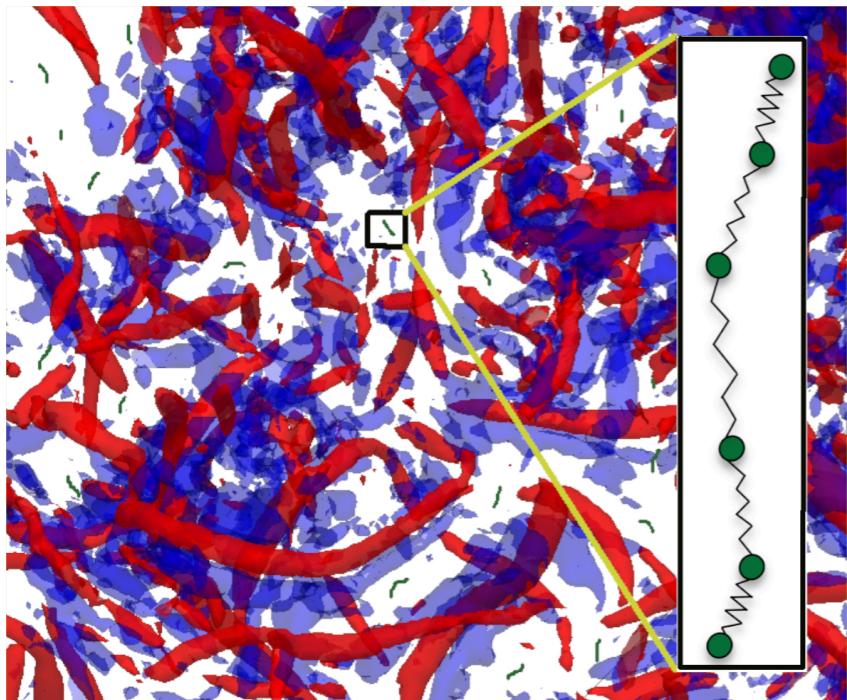
Schroeder, Shaqfeh & Chu
Macromolecules (2004)

Single polymer dynamics in laminar flows

References

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- Shaqfeh, *J. Non-Newtonian Fluid Mech.* (2005)
- Nguyen & Kausch (eds.), *Flexible Polymer Chain Dynamics in Elongational Flow* (Springer, 1999)

Turbulent flows



Lumley, *Symp. Math.* (1972); *J. Polym. Sci.: Macromol. Rev.* (1973)

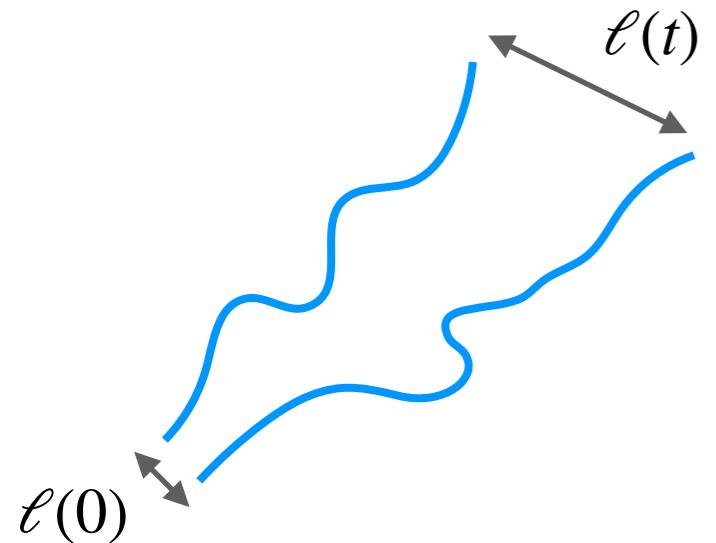
$$\langle R^2 \rangle \propto \exp \left\{ \left(2\langle S^2 \rangle T_L - \frac{1}{\tau} \right) t \right\}$$

$\langle S^2 \rangle$ mean-square strain rate

T_L Lagrangian correlation time scale of the strain rate

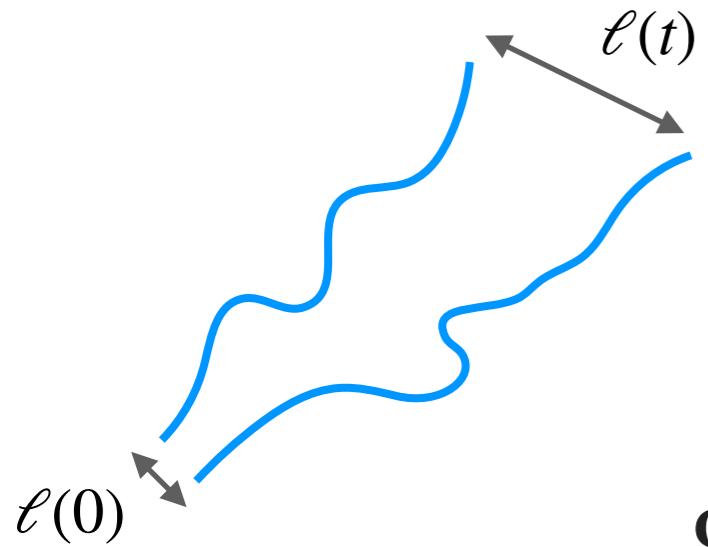
“If the mean-square strain rate exceeds a critical value related to the inverse of the terminal relaxation time but weighted by the persistence of the fluctuating strain rate regions, then the molecules begin to expand exponentially. The expansion of an individual molecule is, of course, not steady; as it moves from region to region, it will first expand, then shrink, etc.; however, when the criterion is exceeded, the expansion will win out, and it will gradually expand more and more.”

Stretching in turbulent flows



Lyapunov exponent $\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \left\langle \ln \left[\frac{\ell(t)}{\ell(0)} \right] \right\rangle$

Stretching in turbulent flows



Lyapunov exponent

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \left\langle \ln \left[\frac{\ell(t)}{\ell(0)} \right] \right\rangle$$

Generalized Lyapunov exponents

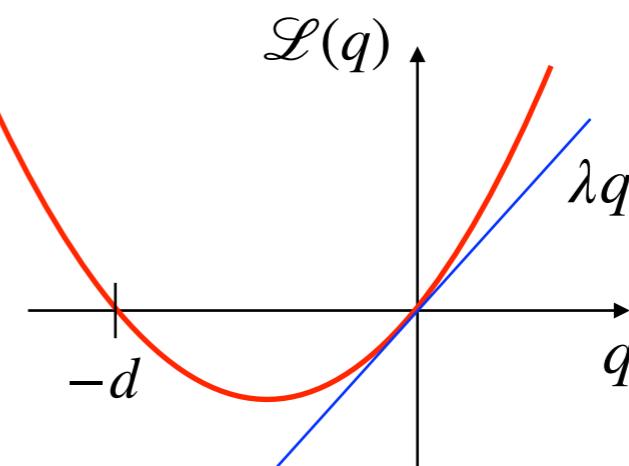
$$\mathcal{L}(q) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \left\langle \left[\frac{\ell(t)}{\ell(0)} \right]^q \right\rangle$$

The function $\mathcal{L}(q)$ is convex and satisfies $\mathcal{L}(-d) = 0$ and $\mathcal{L}'(0) = \lambda$

If the PDF of $\ell(t)$ is log-normal

$$\mathcal{L}(q) = \lambda q + \mu q^2,$$

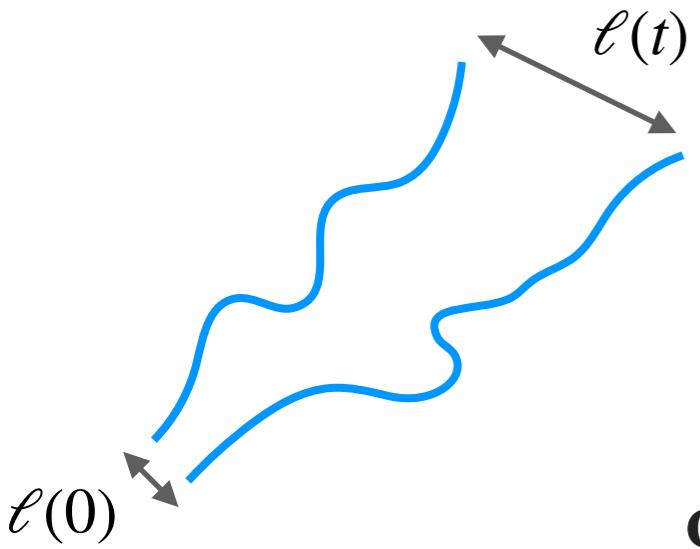
where μ is the variance of $\ln \ell(t)$



Paladin & Vulpiani, *Phys. Rep.* (1987)

Cecconi, Cencini & Vulpiani, *Chaos: from Simple Models to Complex Systems* (World Scientific, 2010)

Stretching in turbulent flows



Lyapunov exponent

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Generalized Lyapunov exponents

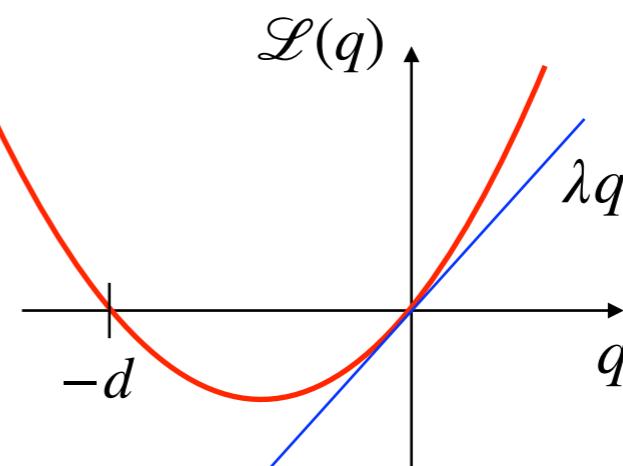
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Cecconi, Cencini & Vulpiani, *Chaos: from Simple Models to Complex Systems* (World Scientific, 2010)

3D turbulent flows

Bec, Biferale, Boffetta, Cencini, Musacchio & Toschi , *Phys. Fluids* (2006)

Bagheri, Mitra, Perlekar & Brandt, *Phys. Rev. E* (2012)

Johnson & Meneveau, *Phys. Fluids* (2016)

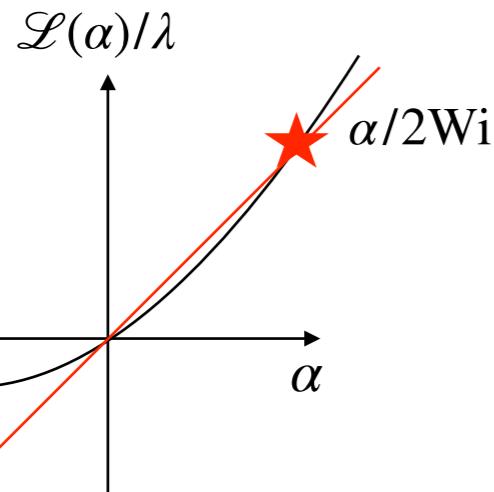
Large deviations theory

Balkovsky, Fouxon & Lebedev, Phys. Rev. Lett. (2000)

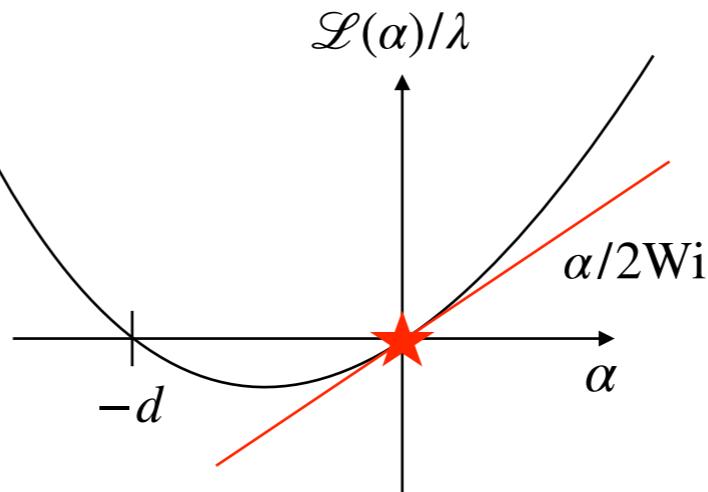
[here we use the formalism of Boffetta, Celani & Musacchio, Phys. Rev. Lett. (2003)]

$$P_{\text{st}}(R) \sim R^{-1-\alpha} \quad \text{for} \quad R_{eq} \ll R \ll L$$

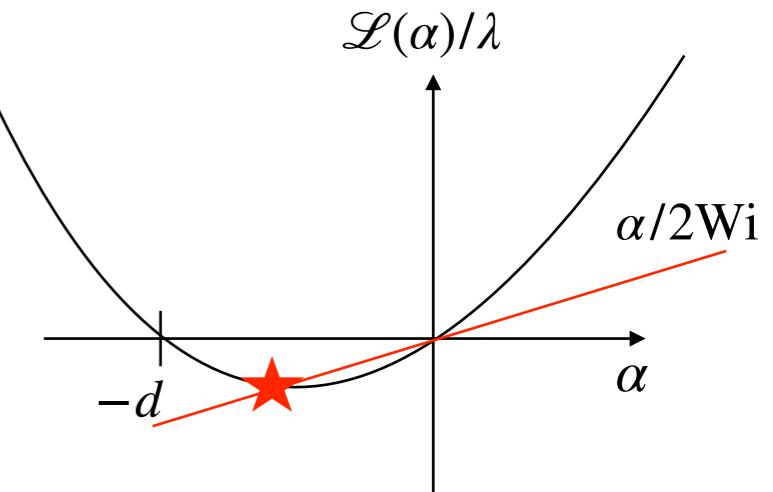
$$\frac{\mathcal{L}(\alpha)}{\lambda} = \frac{\alpha}{2\text{Wi}}, \quad \text{Wi} = \lambda\tau$$



$$\text{Wi} < 1/2 \rightarrow \alpha > 0$$



$$\text{Wi} = 1/2 \rightarrow \alpha = 0$$



$$\text{Wi} > 1/2 \rightarrow \alpha < 0$$

For $\text{Wi} = 1/2$ and $L \rightarrow \infty$, the PDF of R ceases to be normalisable \implies Coil–stretch transition at $\text{Wi}_{\text{crit}} = 1/2$

Near Wi_{crit} the log-normal approximation $\mathcal{L}(q) = \lambda q + \mu q^2 + O(q^3)$ yields $\alpha = \frac{\lambda}{\mu} \left(\frac{1}{\text{Wi}} - 2 \right)$

Batchelor—Kraichnan random flow

FENE dumbbell model

stochastic differential equation

$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \boldsymbol{\xi}(t), \quad f(R) = \frac{1}{1 - R^2/L^2}$$

Fokker–Planck equation for $\psi(\mathbf{R}, t)$

$$\partial_t \psi = - \nabla_{\mathbf{R}} \cdot \left\{ \left[\nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} \right] \psi \right\} + \frac{R_{eq}^2}{2\tau} \Delta_{\mathbf{R}} \psi$$

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Kraichnan flow (Batchelor regime): $\nabla \mathbf{u}$ is a $d \times d$ -dimensional isotropic white noise

$$\langle \nabla_j u_i(t) \nabla_l u_k(t') \rangle = \mathcal{K}_{ijkl} \delta(t - t'), \quad \mathcal{K}_{ijkl} = 2\lambda[(d+1)\delta^{ik}\delta^{jl} - \delta^{ij}\delta^{kl} - \delta^{il}\delta^{jk}] / d(d-1)$$

Falkovich, Gawedzki & Vergassola, *Rev. Mod. Phys.* (2001)

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Falkovich, Gawedzki & Vergassola, *Rev. Mod. Phys.* (2001)

PDF of R with respect to both thermal noise and $\nabla \mathbf{u}$: $P(R, t)$

Thanks to isotropy,
1D Fokker–Planck eq.

$$\partial_t P = - \partial_R [D_1(R)P] + \partial_R^2 [D_2(R)P]$$

$$D_1(R) = \frac{2(d+1)}{d} \text{Wi} R - f(R)R + (d-1) \frac{R_{eq}^2}{R}$$

$$D_2(R) = \frac{2\text{Wi}}{d} + R_{rq}^2$$

Batchelor—Kraichnan random flow

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stochastic differential equation

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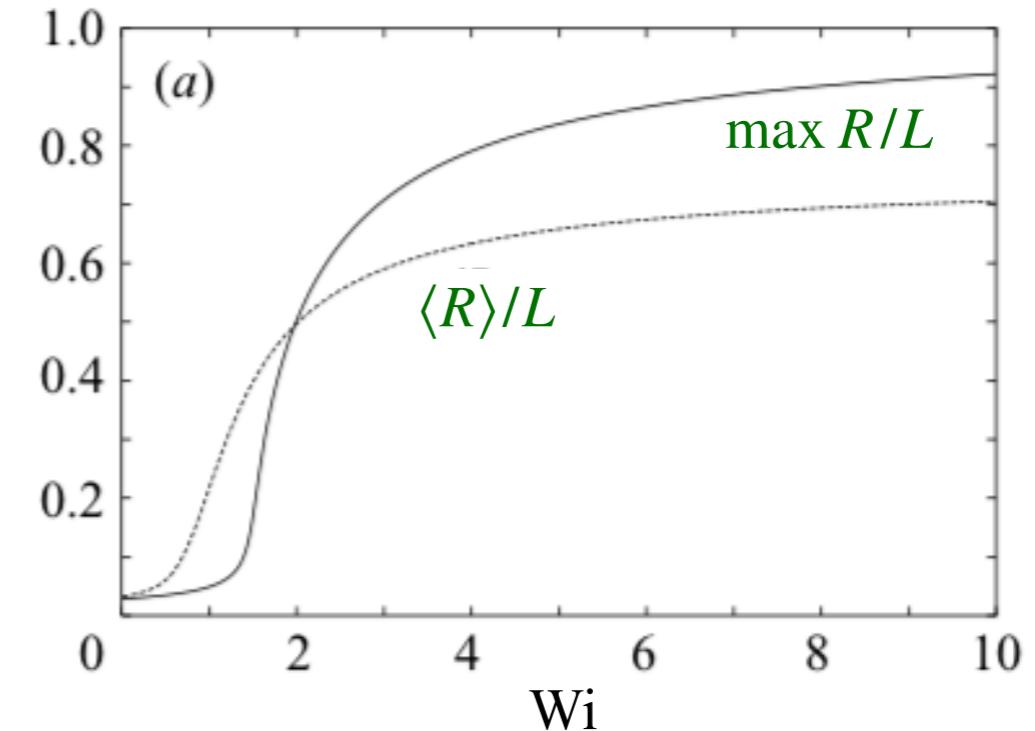
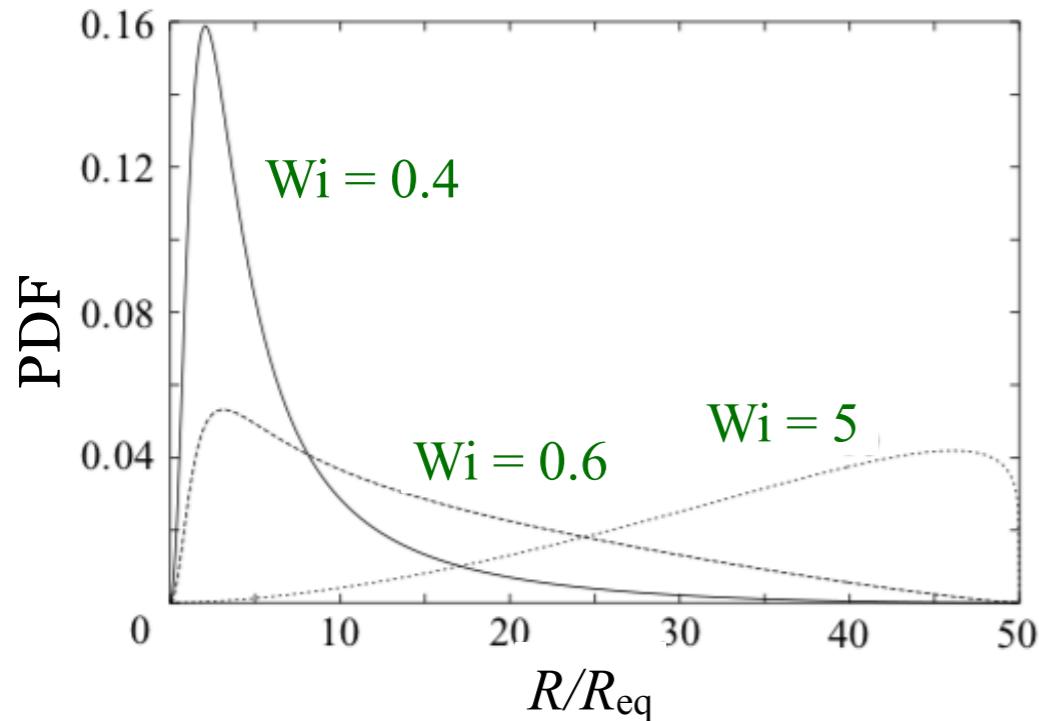
$$P_{\text{st}}(R) \propto R^{d-1} \left(1 + \frac{2\text{Wi}}{d} \frac{R^2}{R_{eq}^2} \right)^{-h} \left(1 - \frac{R^2}{L^2} \right)^h \quad h = [2(b^{-1} + 2\text{Wi}/d)]^{-1}$$

For $R_{eq} \ll R \ll L$: $P_{\text{st}}(R) \sim R^{-1-\alpha}$ with $\alpha = d \left(\frac{1}{2\text{Wi}} - 1 \right)$

In the Batchelor–Kraichnan flow, the statistics of $\ell(t)$ is log-normal with $\lambda/\mu = d$

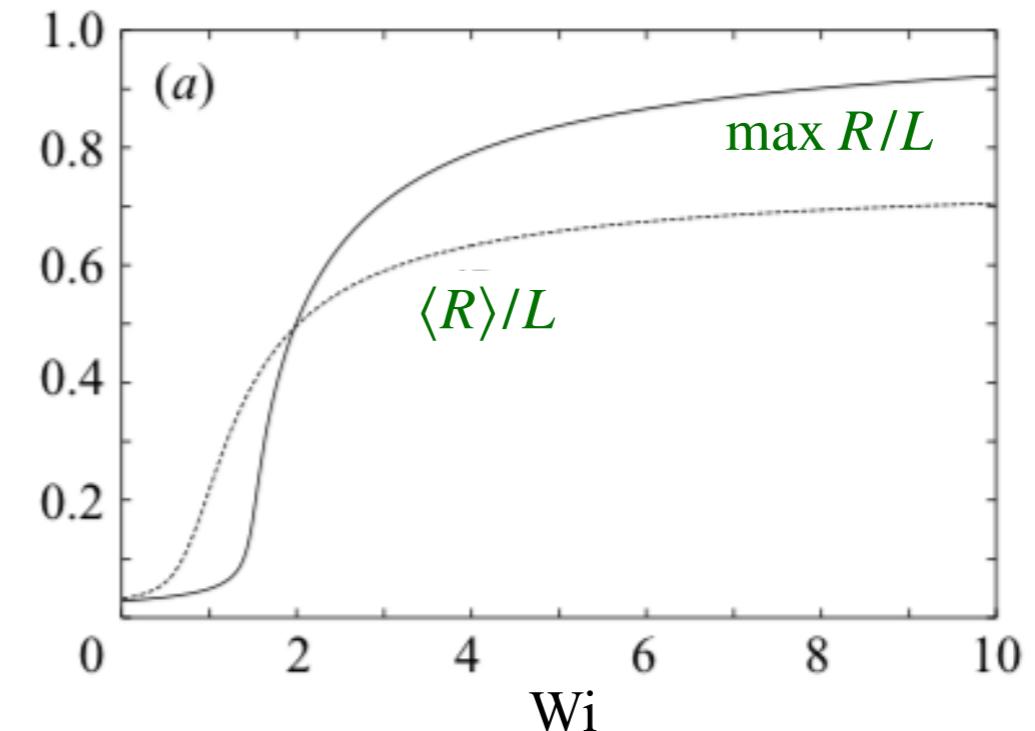
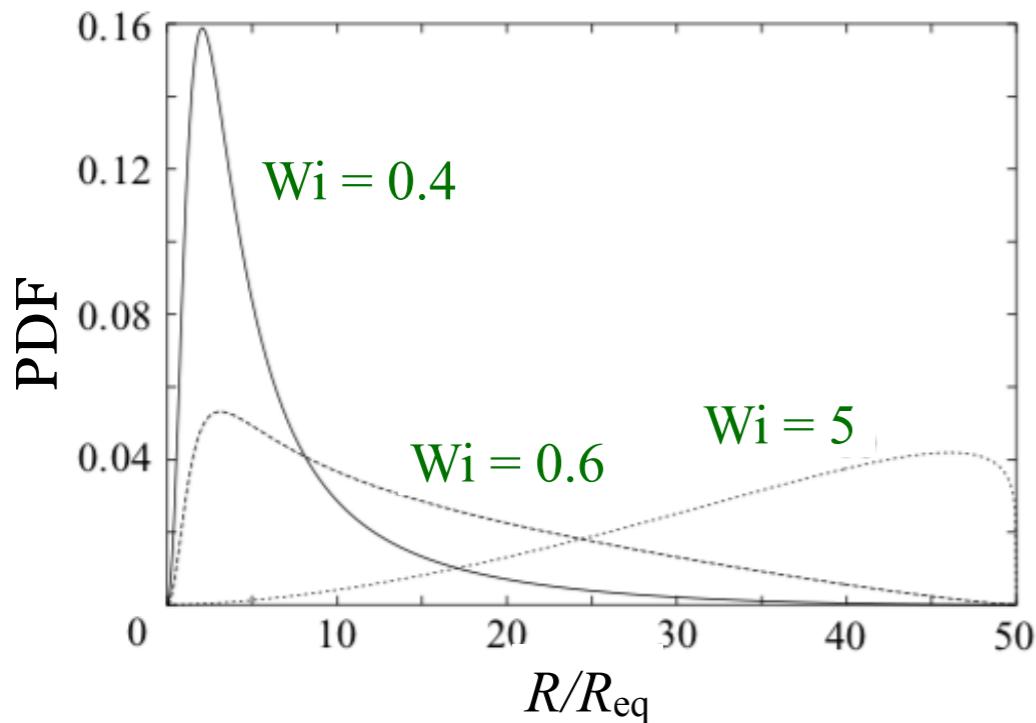
Martins Afonso & DV, *J. Fluid Mech.* (2005)

Batchelor—Kraichnan random flow



Martins Afonso & DV, *J. Fluid Mech.* (2005)

Batchelor—Kraichnan random flow



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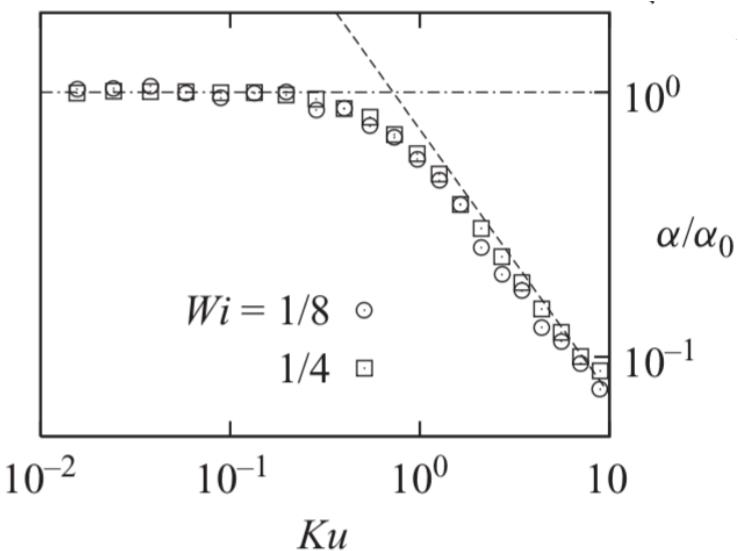
Polymers in the Batchelor—Kraichnan flow

- Chertkov, *Phys. Rev. Lett.* (2000)
- Thiffeault, *Phys. Lett. A* (2003)
- Celani, Musacchio & DV, *J. Stat. Phys.* (2005)
- Celani, Puliafito & DV, *Phys. Rev. Lett.* (2006)
- Plan, Ali & DV, *Phys. Rev. E* (2016)

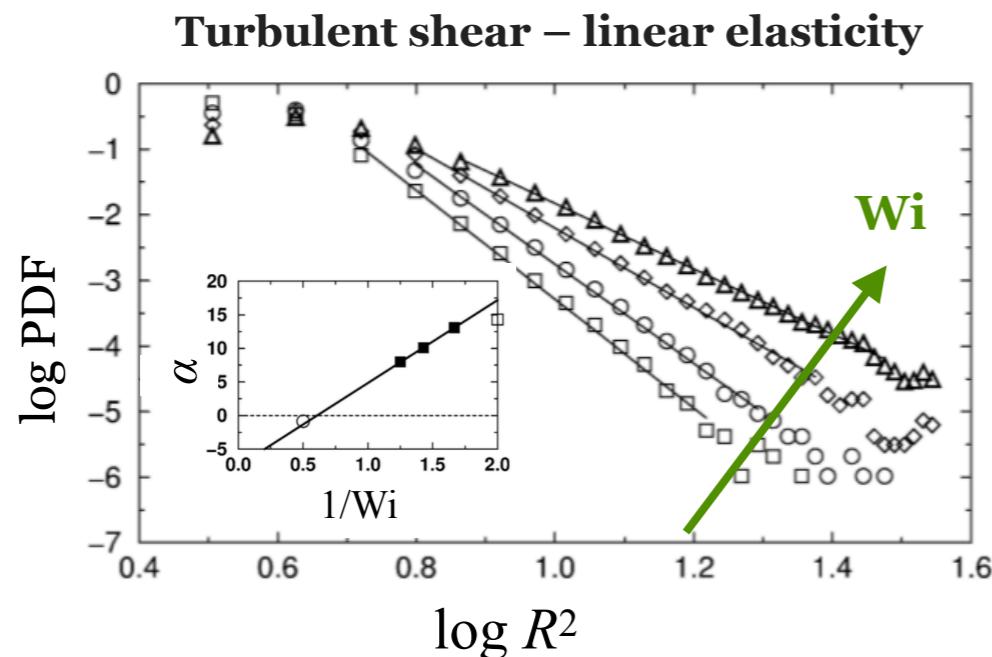
2D random renewing flow

$$\begin{aligned} Ku &= \lambda T_{\text{corr}} \\ \alpha_0 &= \alpha(Ku = 0) \end{aligned}$$

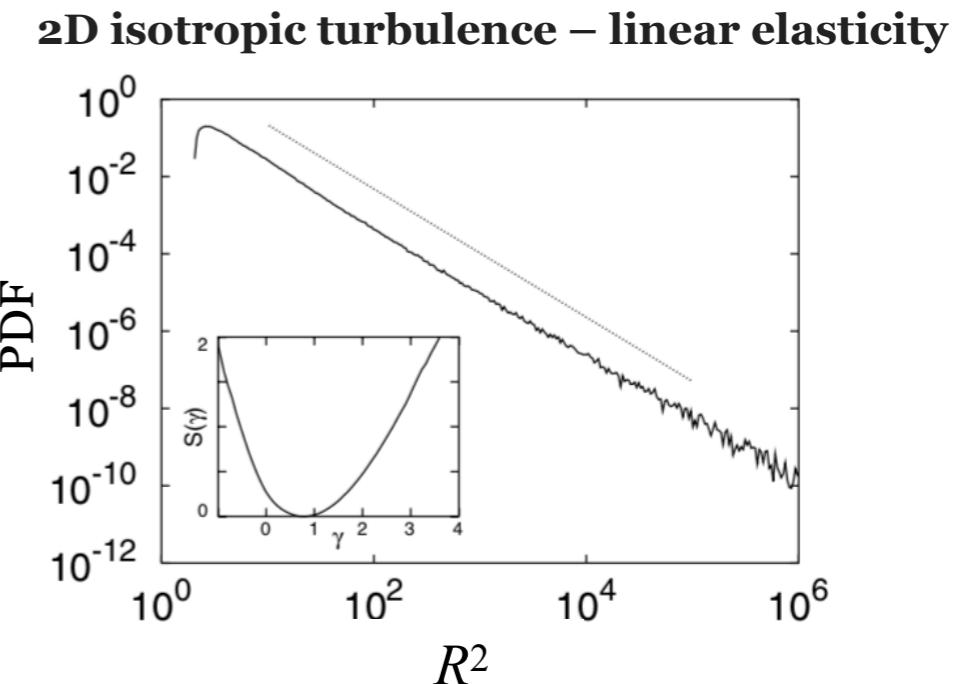
Musacchio & DV, *J. Fluid Mech.* (2011)



Numerical simulations

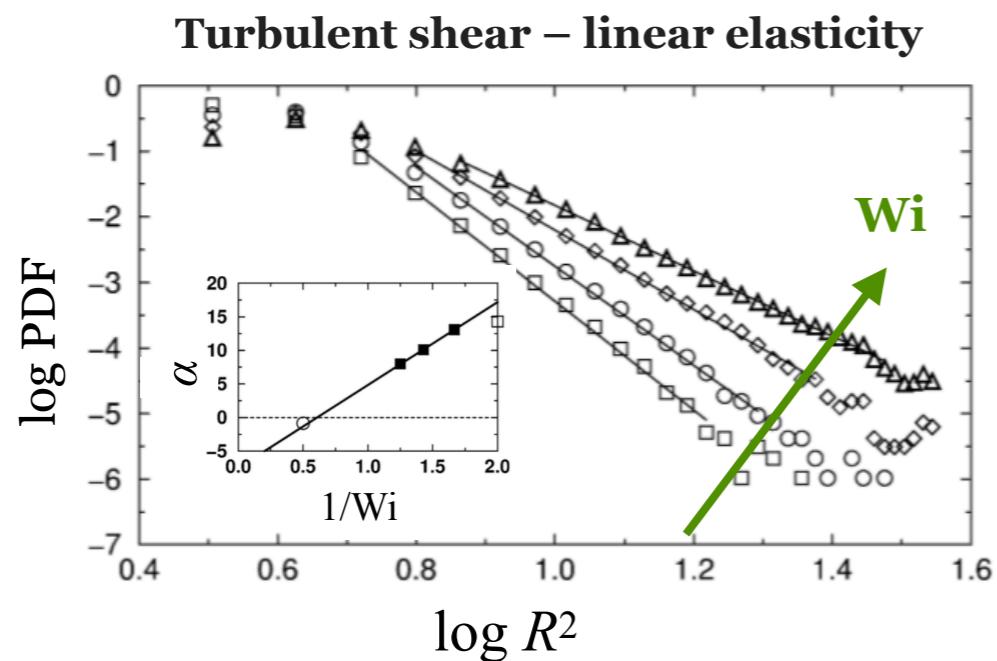


Eckhardt, Kronjäger & Schumacher, *Comput. Phys. Commun.* (2002)

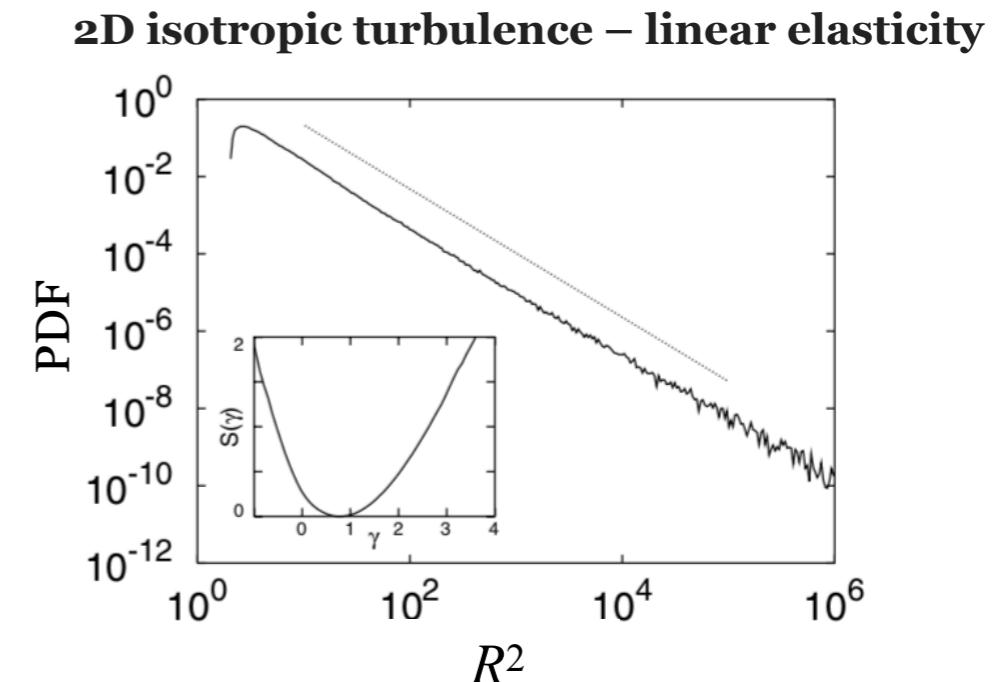


Boffetta, Celani & Musacchio, *Phys. Rev. Lett.* (2003)

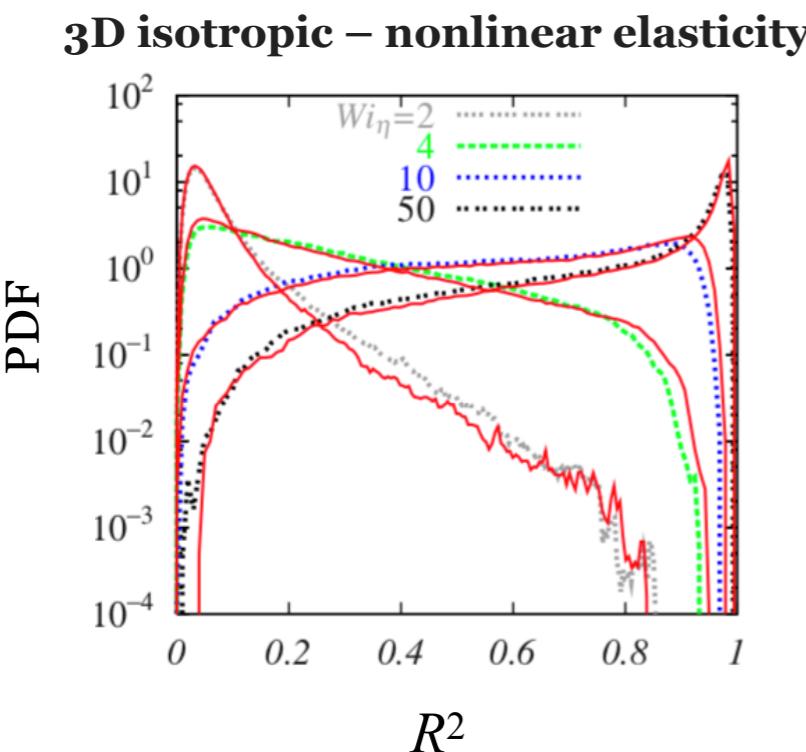
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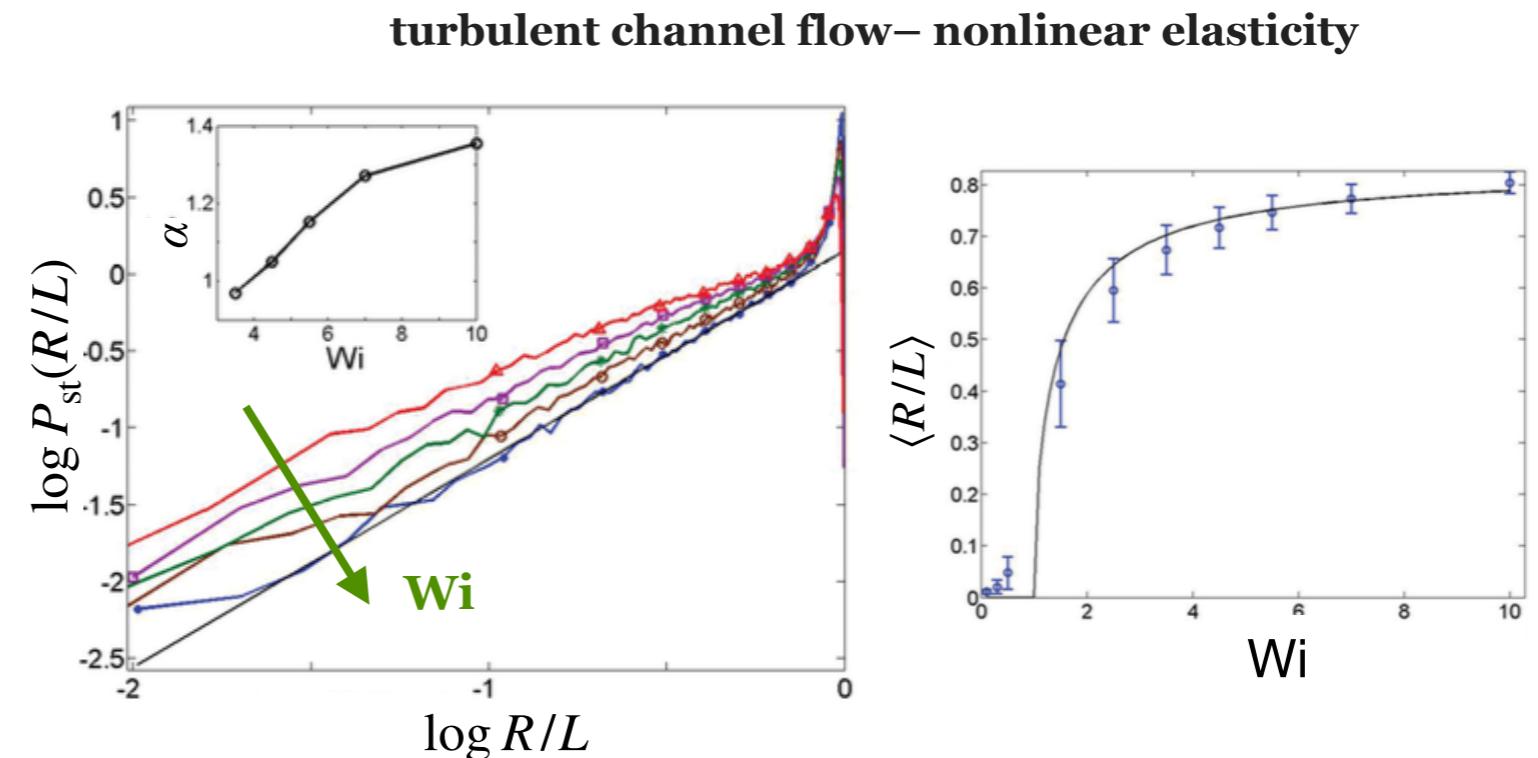
Eckhardt, Kronjäger & Schumacher, *Comput. Phys. Commun.* (2002)



Boffetta, Celani & Musacchio, *Phys. Rev. Lett.* (2003)

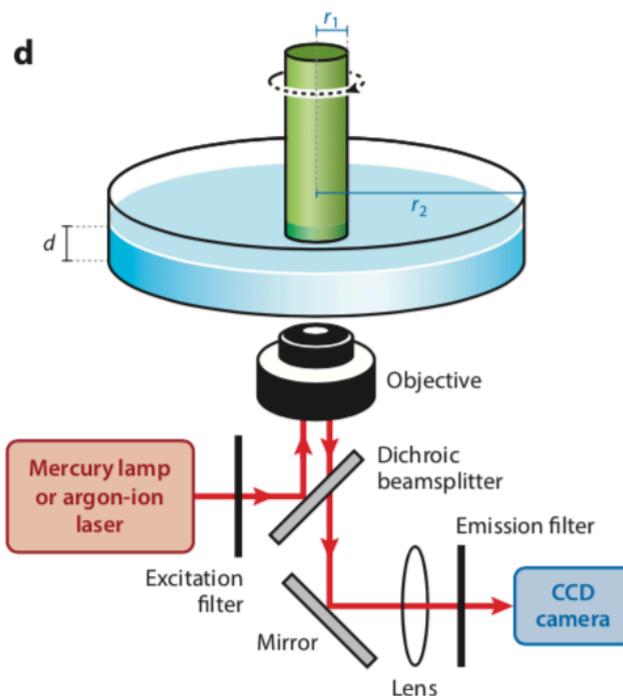


Watanabe & Gotoh, *Phys. Rev. E* (2010)



Bagheri, Mitra, Perlekar & Brandt, *Phys. Rev. E* (2012)

Experiments

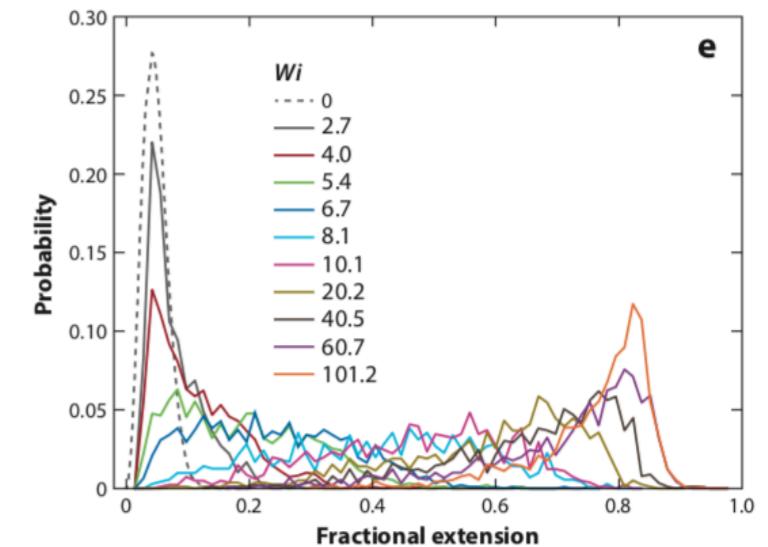


$$r_1 = 2.25\text{mm}, r_2 = 6\text{mm}$$
$$d = 675\mu\text{m}$$

λ DNA
($R_g = 0.73\mu\text{m}$, $L = 21\mu\text{m}$)

T4 DNA
($R_{eq} = 3\mu\text{m}$, $L = 71.7\mu\text{m}$)

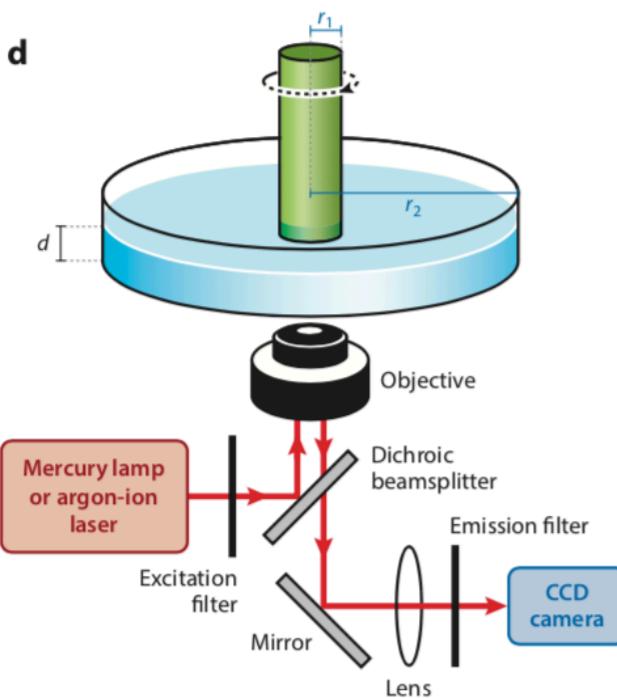
Reynolds < 1



Chevallard, Gerashchenko & Steinberg, *EPL* (2005)
Steinberg, *C.R. Physique* (2009)
Liu & Steinberg, *EPL* (2010)

Liu & Steinberg, *Macromol. Symp.* (2014)
Steinberg, *Annu. Rev. Fluid Mech.* (2021)

Experiments



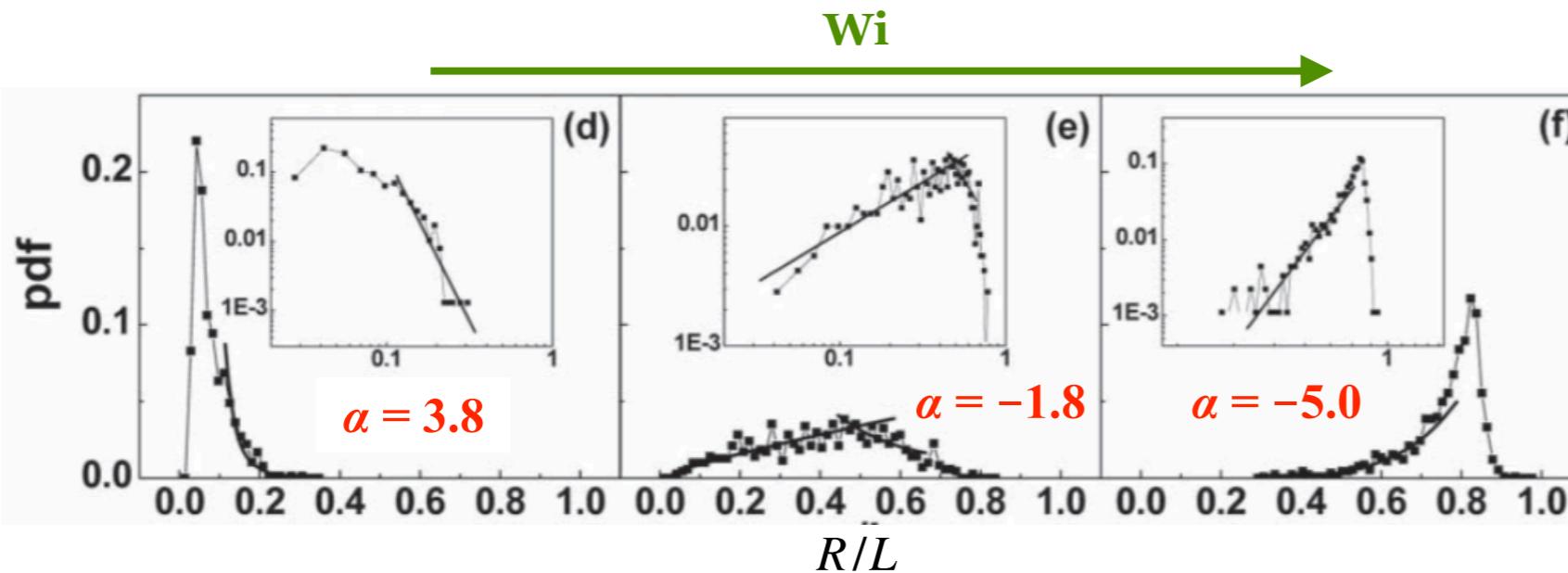
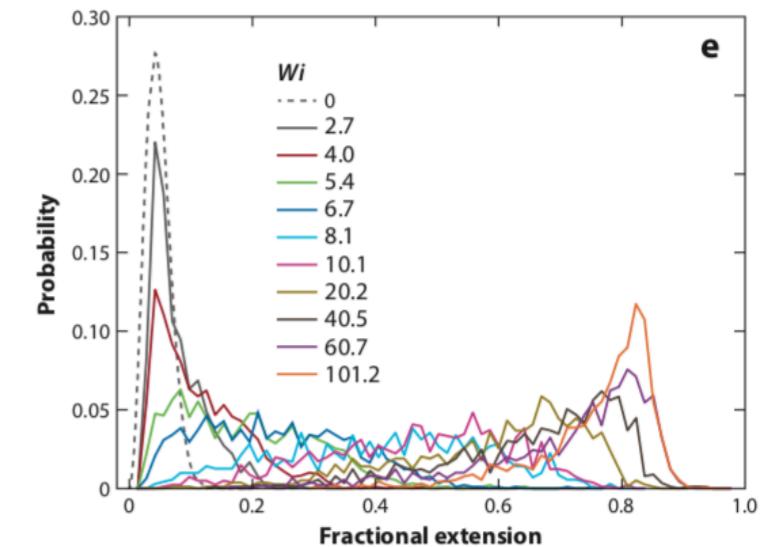
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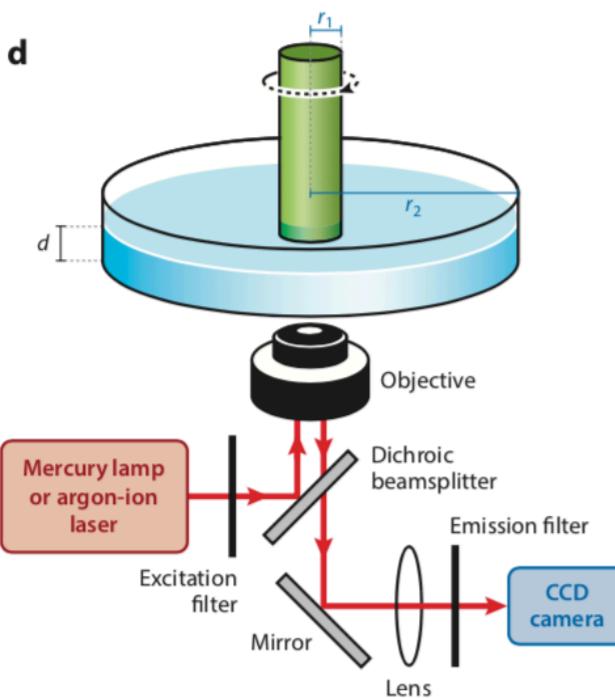
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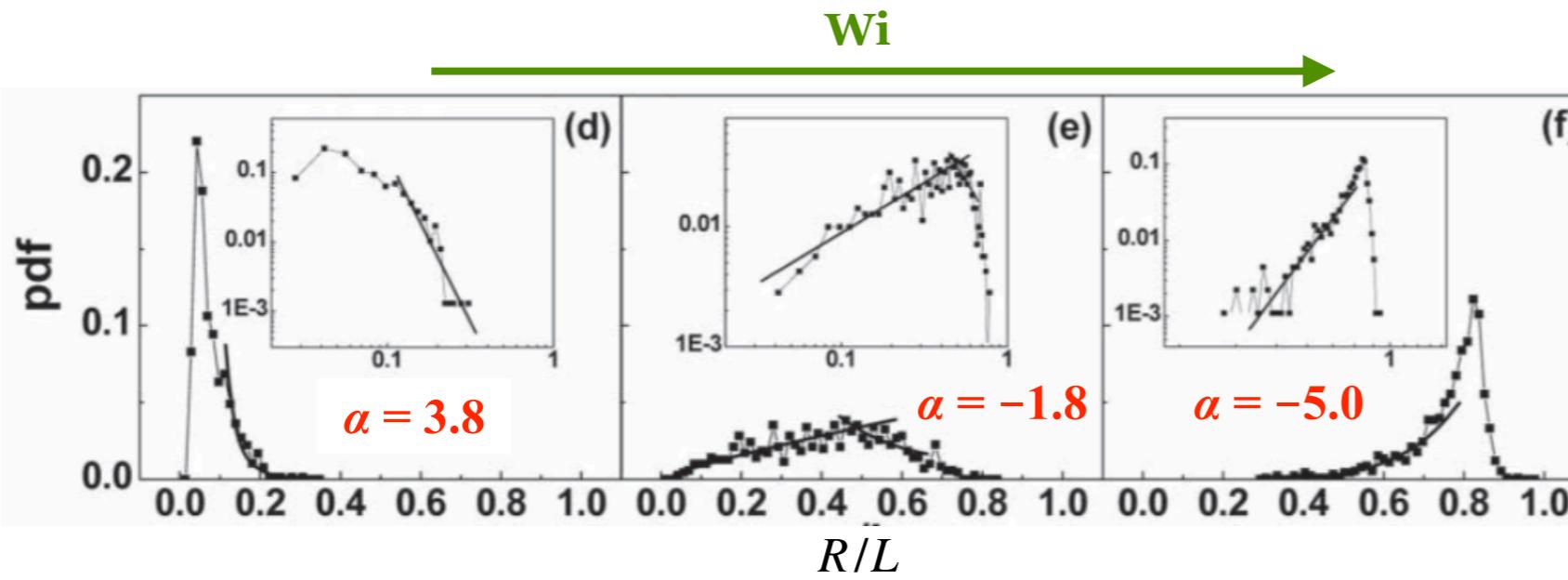
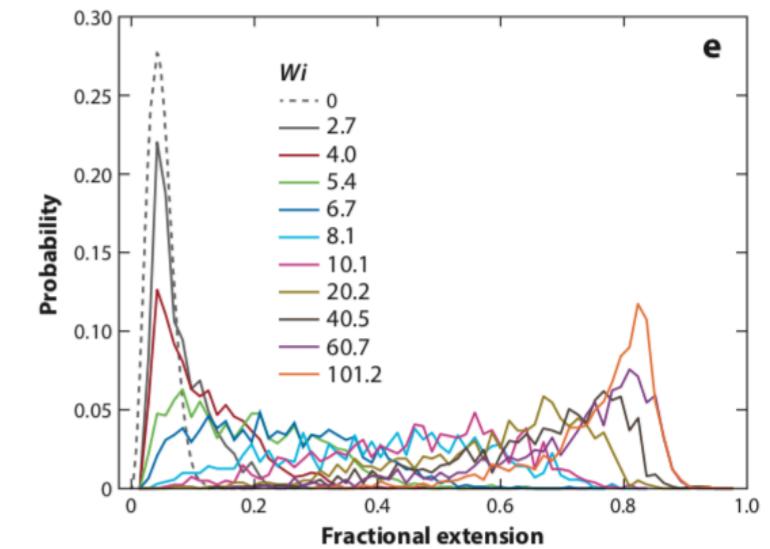
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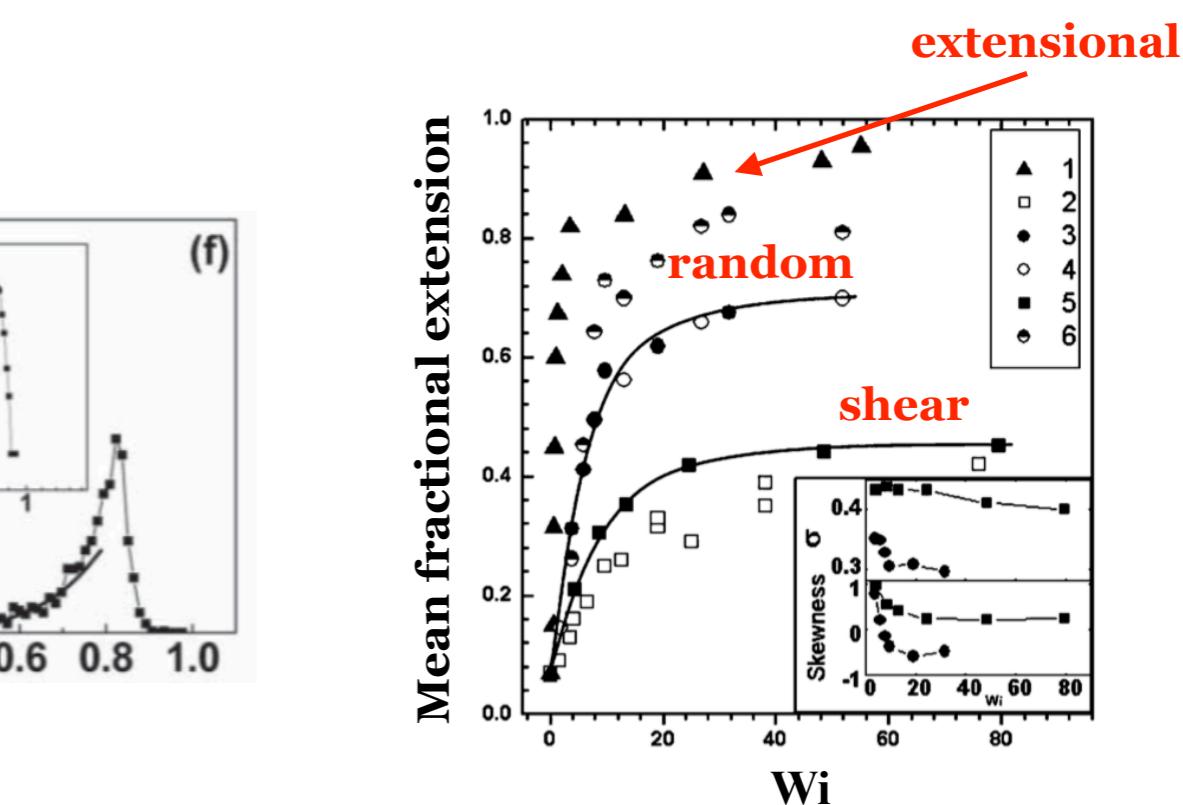
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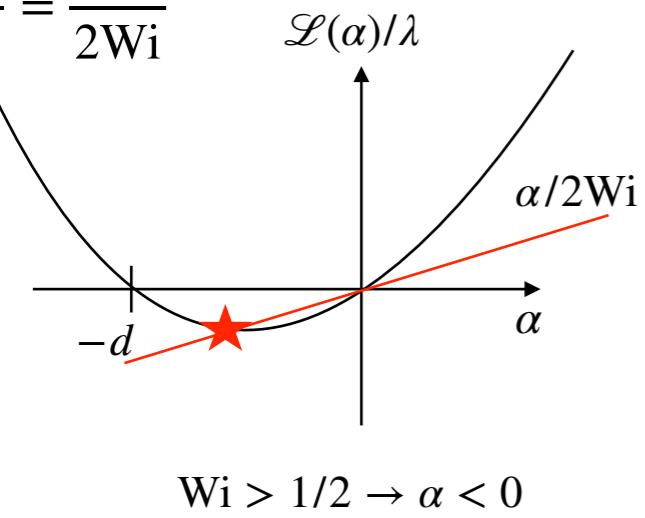
Chevallard, Gerashchenko & Steinberg, *EPL* (2005)
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Liu & Steinberg, *Macromol. Symp.* (2014)
Steinberg, *Annu. Rev. Fluid Mech.* (2021)

Effect of internal viscosity

$$\frac{\mathcal{L}(\alpha)}{\lambda} = \frac{\alpha}{2\text{Wi}}$$



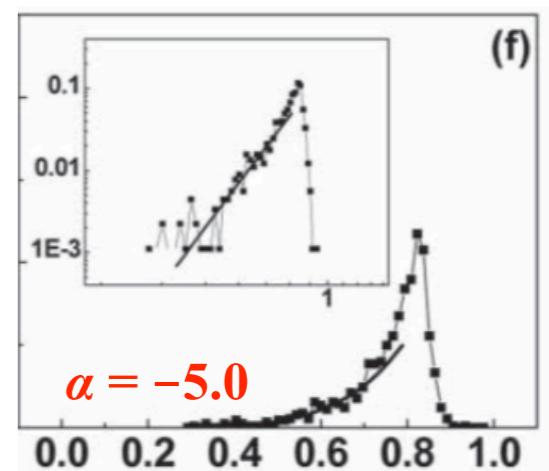
Theory

$$P_{\text{st}}(R) \sim R^{-1-\alpha} \quad (R_{eq} \ll R \ll L)$$

$$\lim_{\text{Wi} \rightarrow \infty} \alpha = -d$$

$$\text{At large Wi: } P_{\text{st}}(R) \sim R^{d-1}$$

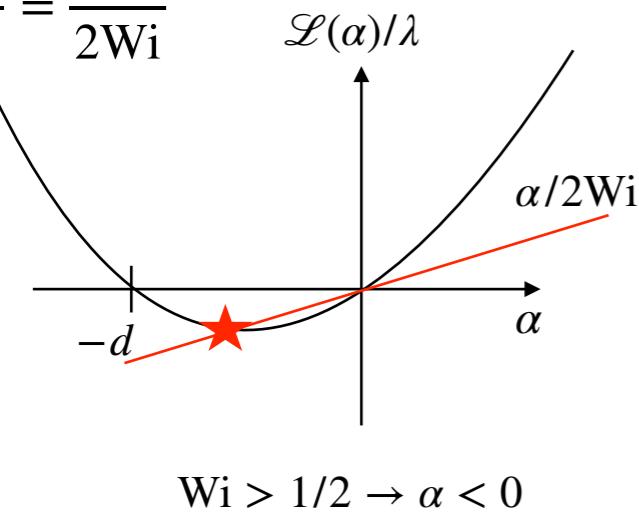
Experiment at large Wi:
 $P_{\text{st}}(R) \sim R^4$



Liu & Steinberg, *Macromol. Symp.* (2014)

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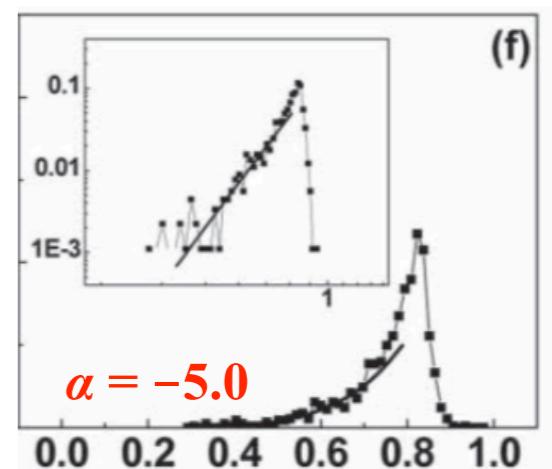
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Liu & Steinberg, *Macromol. Symp.* (2014)

Internal viscosity



Kuhn & Kuhn, *Helv. Chim. Acta* (1945)

$$\mathbf{F}^{\text{iv}} = -\phi(\mathbf{R} \cdot \dot{\mathbf{R}}) \frac{\mathbf{R}}{R^2}$$

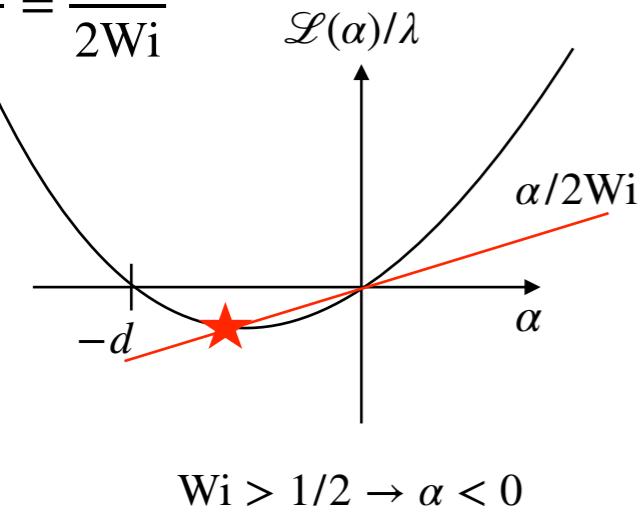
internal viscosity parameter

$$\epsilon = \frac{2\phi}{\zeta}$$

For recent applications: Kailasham, Chakrabarti & Prakash
J. Chem. Phys. (2018); *Phys. Rev. Res.* (2020)

Effect of internal viscosity

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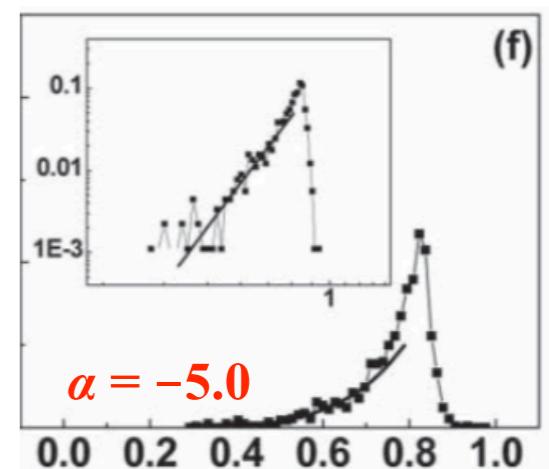
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$$\mathbf{F}^{\text{iv}} = -\phi(\mathbf{R} \cdot \dot{\mathbf{R}}) \frac{\mathbf{R}}{R^2}$$

internal viscosity parameter

$$\epsilon = \frac{2\phi}{\zeta}$$

$$\frac{1}{\lambda} \mathcal{L}\left(\frac{\alpha_\epsilon}{1+\epsilon}\right) = \frac{\alpha_\epsilon}{2(1+\epsilon)\text{Wi}}$$

$$\alpha_\epsilon = \alpha(1+\epsilon)$$

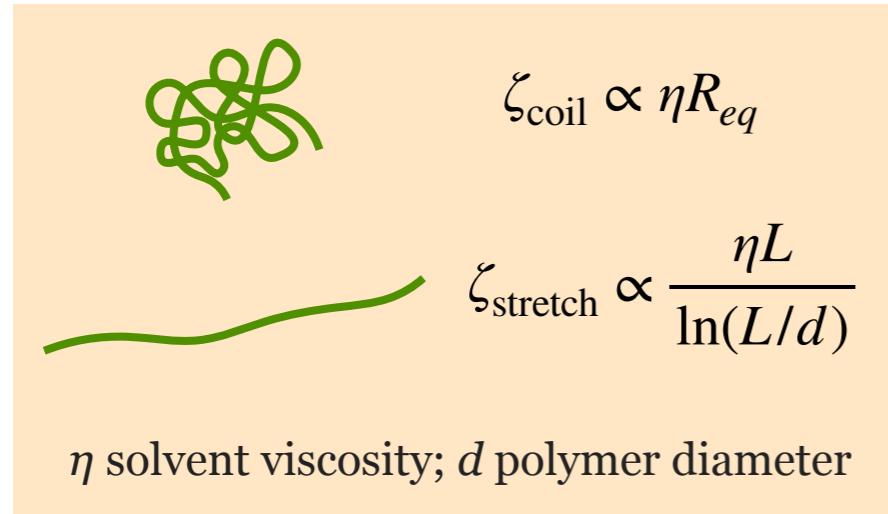
$$\text{At large Wi: } P_{\text{st}}(R) \sim R^{d(1+\epsilon)-1}$$

$$\text{For } \epsilon = 2/3, \quad P_{\text{st}}(R) \sim R^4$$

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DV, *Soft Matter* (2021)

Temporal dynamics – Relaxation to steady state

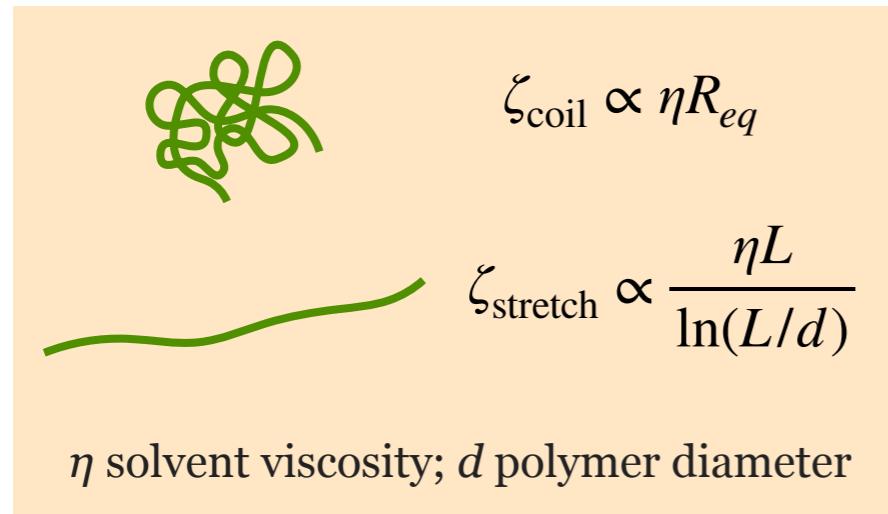


Conformation-dependent drag (Hinch, 1975)

$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau \nu(R)} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \xi(t)$$

$$\tau = \zeta_c / 4k, \quad \nu(R) = 1 + (\zeta_s / \zeta_c - 1)R/L$$

Temporal dynamics – Relaxation to steady state



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$$\tau = \zeta_c / 4k, \quad \nu(\mathbf{R}) = 1 + (\zeta_s / \zeta_c - 1) R / L$$

Batchelor–Kraichan flow

Expansion into eigenfunctions of the FP operator

$$\partial_t P = - \partial_R [D_1(R)P] + \partial_R^2 [D_2(R)P]$$

$$P(R, t) = P_{\text{st}}(R) + \sum_{n=1}^{\infty} a_n p_n(r) e^{-\sigma_n t}$$

$p_n(r)$ are the eigenfunctions of the FP operator and σ_n ($\sigma_n < \sigma_{n+1}$) the associated eigenvalues

$$T_{eq} = \sigma_1^{-1}$$

Temporal dynamics – Relaxation to steady state

Batchelor–Kraichnan flow

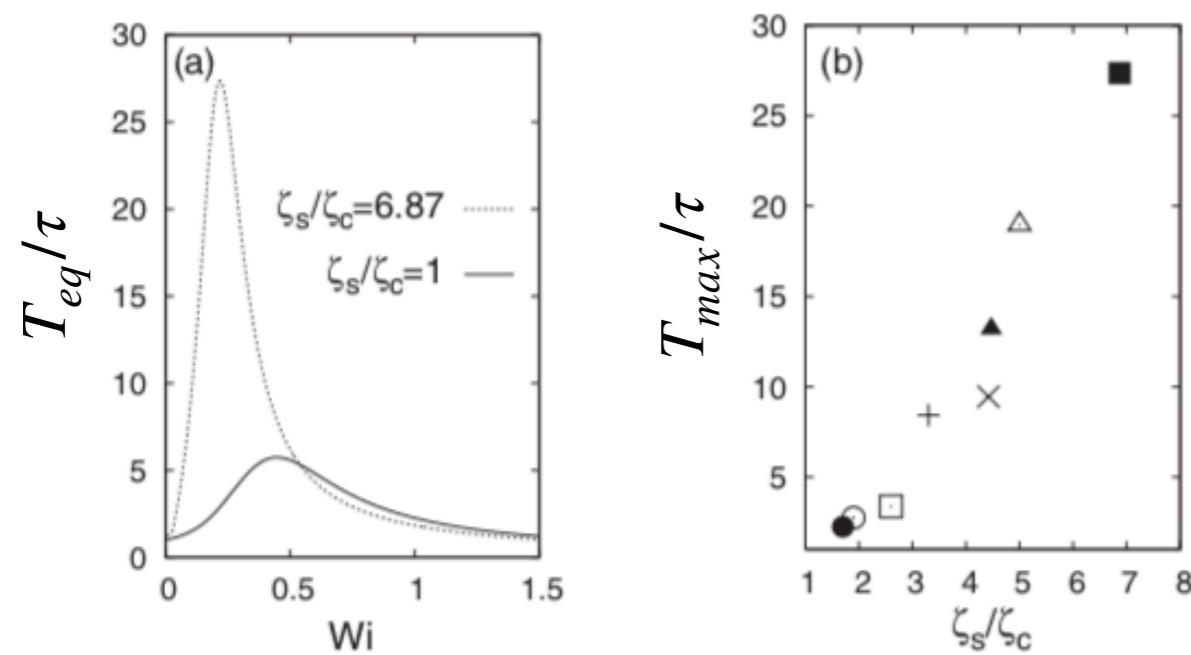
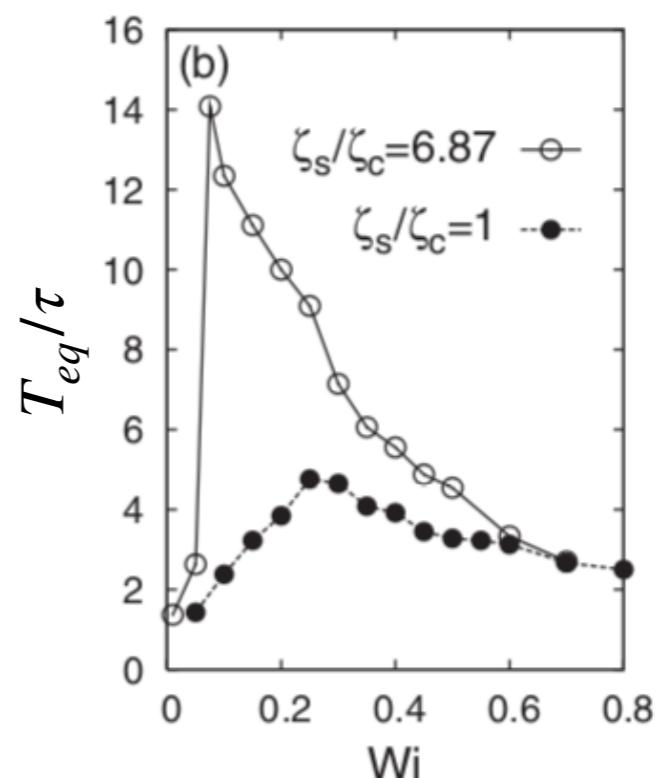


FIG. 3. Three-dimensional Batchelor-Kraichnan flow: (a) t_{rel}/τ vs Wi for a PAM molecule ($b = 3953$); (b) t_{max}/τ for the following polymers: DNA (\bullet , $b = 191.5$; \circ , $b = 260$; \square , $b = 565$; $+$, $b = 2250$), polystyrene (\times , $b = 673$), polyethyleneoxide (PEO) (\blacktriangle , $b = 1666$), *Escherichia Coli* DNA (\triangle , $b = 9250$), and PAM (\blacksquare). Measures of b and ζ_s/ζ_c can be found in

stochastic flow with nonzero correlation time



Temporal dynamics – Relaxation to steady state

Batchelor–Kraichnan flow

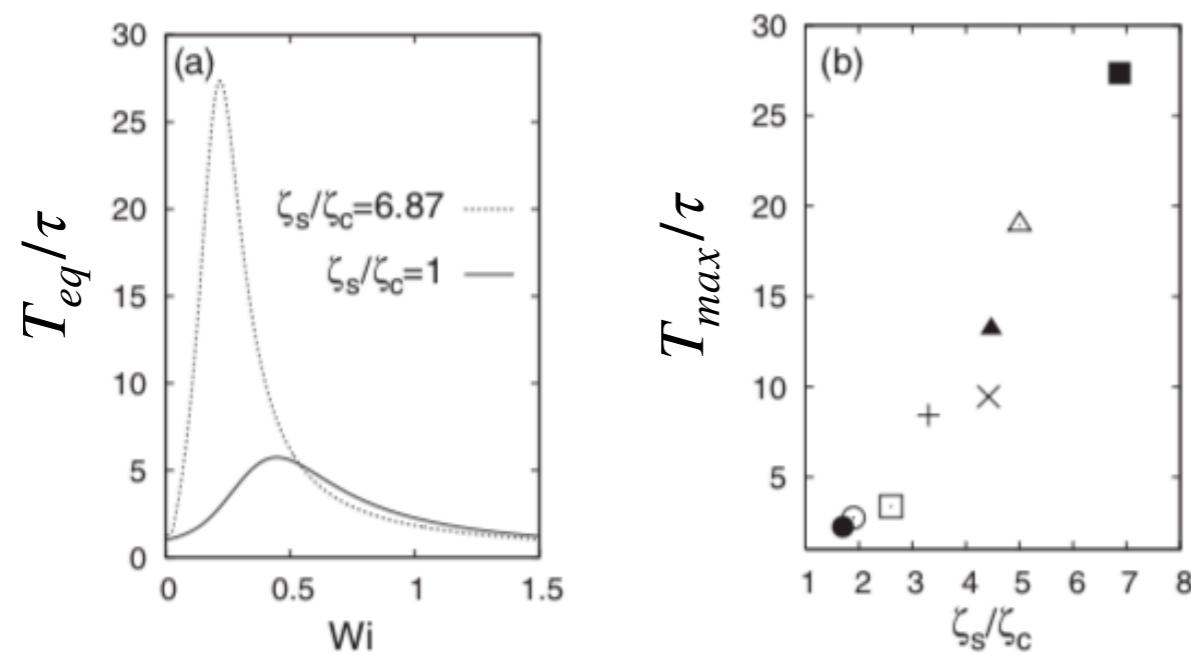
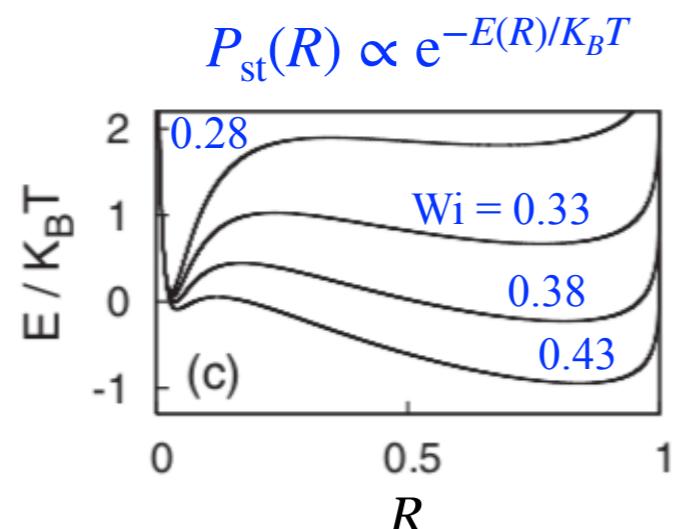
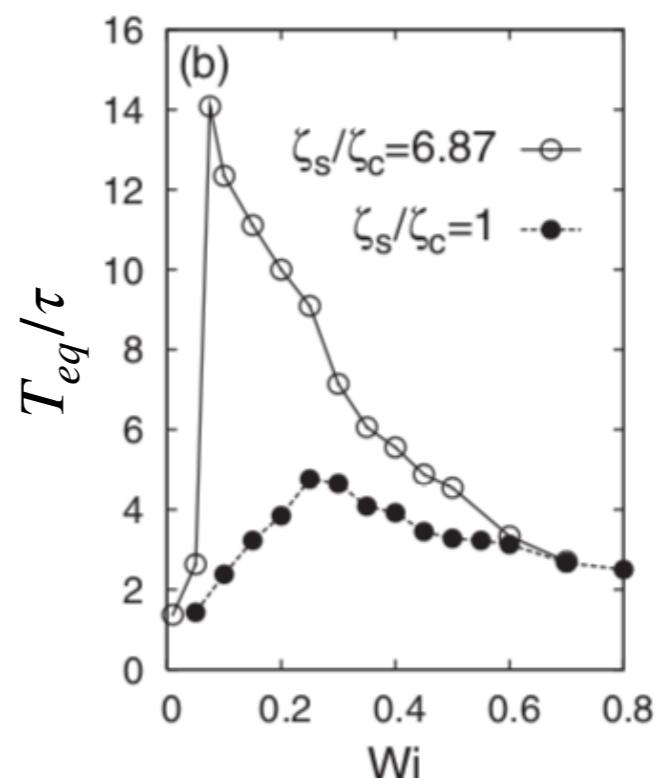


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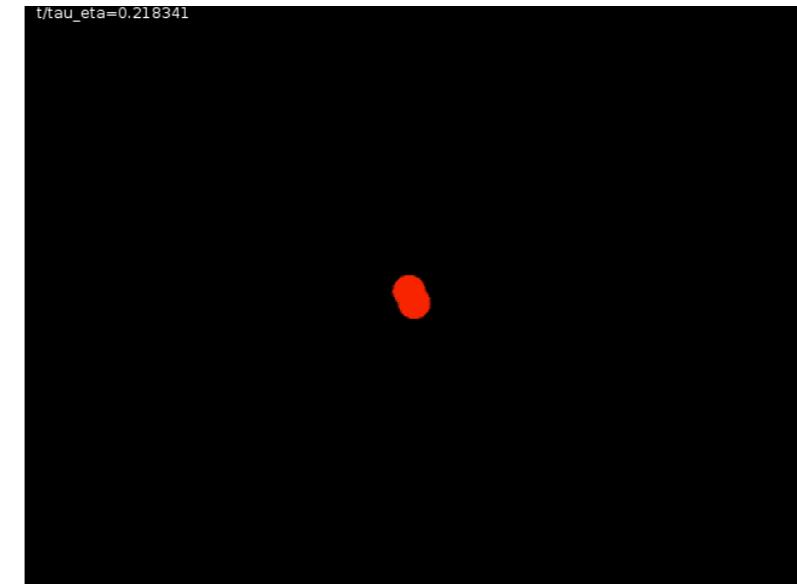
stochastic flow with nonzero correlation time



- The slowing down of the dynamics is due to the heterogeneity of configurations near the CS transition
- No hysteresis is observed

Validity of the dumbbell model

DNS of 3D isotropic turbulence at $R_\lambda = 65$



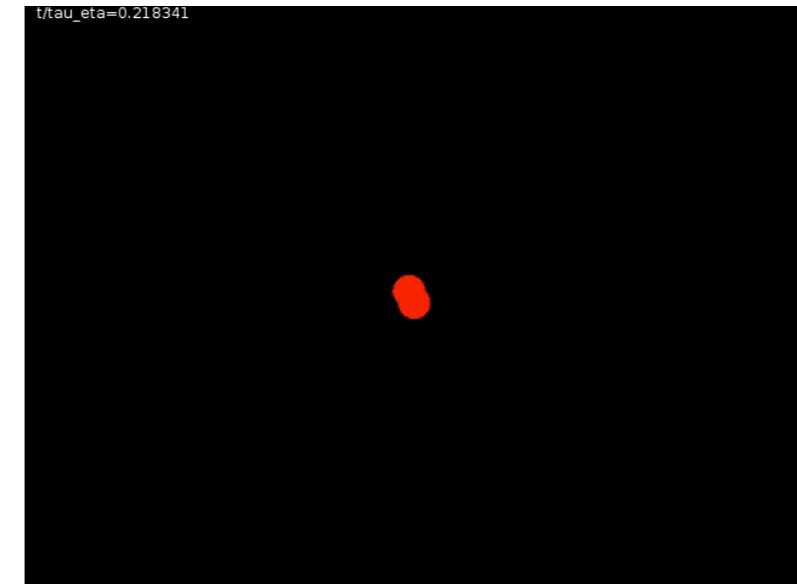
Parameter mapping (Jin & Collins, *New J. Phys.*, 2007)

N number of beads

$$L_{\text{chain}}^2 = \frac{L_{\text{dumb}}^2}{N - 1} \quad \tau_{\text{chain}} = \frac{6\tau_{\text{dumb}}}{N(N + 1)}$$

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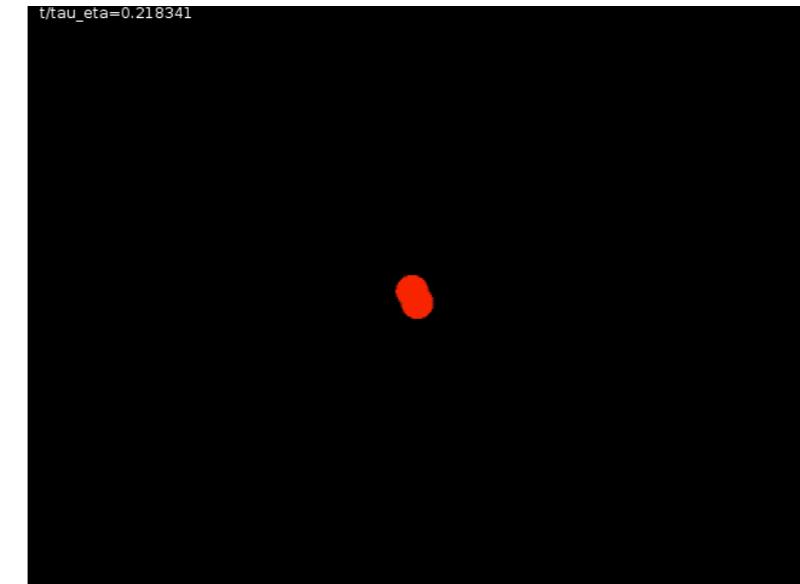
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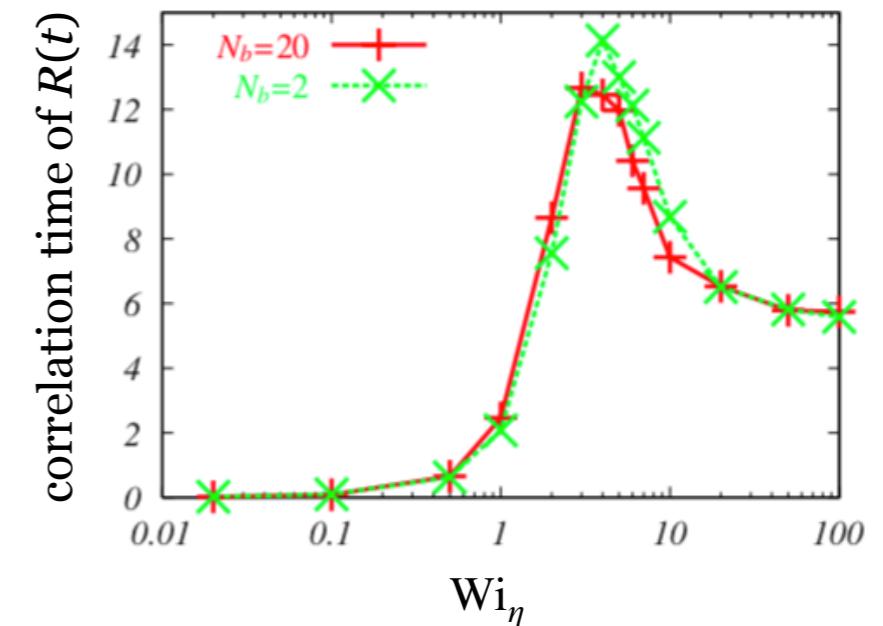
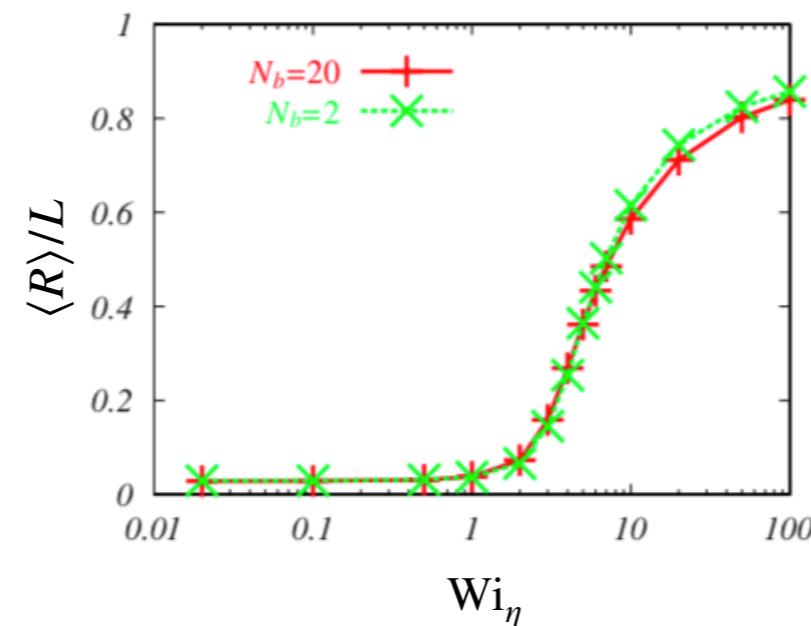
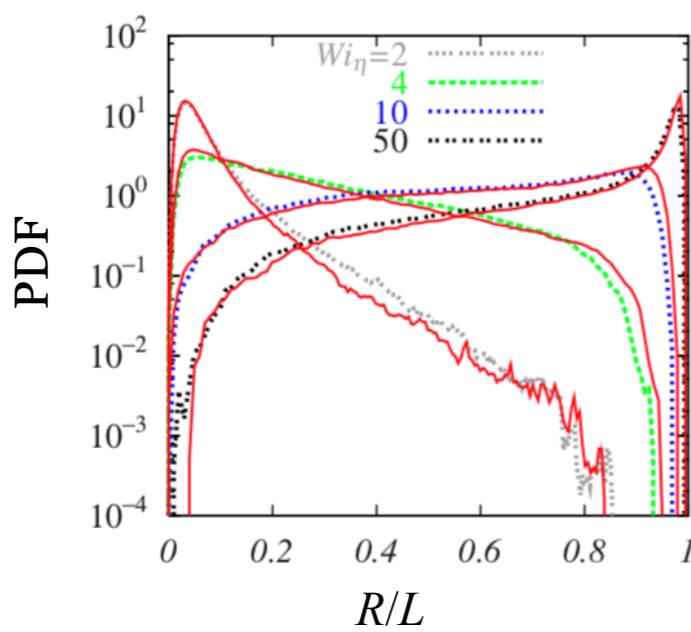
$$N \text{ number of beads}$$

$$L_{\text{chain}}^2 = \frac{L_{\text{dumb}}^2}{N - 1} \quad \tau_{\text{chain}} = \frac{6\tau_{\text{dumb}}}{N(N + 1)}$$

Comparison between a chain ($N=20$, red curves) and a dumbbell ($N=2$)

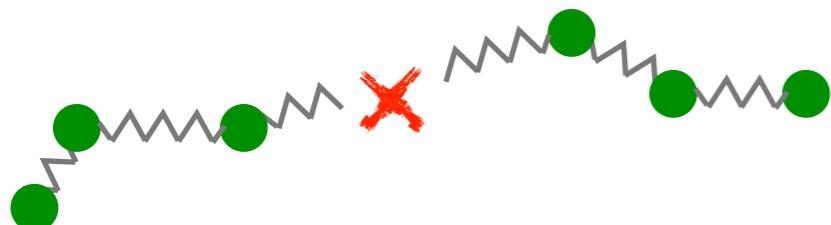
(Watanabe & Gotoh, *Phys. Rev. E*, 2010)

Lagrangian simulation in 3D isotropic turbulence at $R_\lambda = 47$ with 256 polymers



Breakup statistics

When the tension in one of the elastic links exceeds a critical value, the link breaks

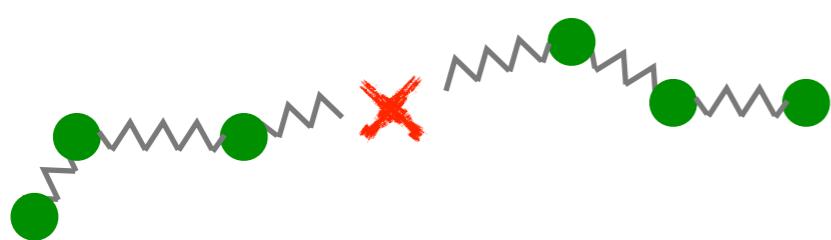


$$|F_i^{\text{el}}| = \frac{R_i}{1 - R_i^2/\ell^2} \geq \mathcal{F}_{\text{break}} \quad \text{equivalent to: } R_i \geq R_{\text{break}}$$

$$R_{eq} \leq R_0 \leq R_{\text{break}} \leq L \leq \eta_K \quad R_0 = R(0)$$

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Dumbbell model in the Batchelor–Kraichnan flow

$P(R, t)$ pdf of the extension: $\partial_t P = -\partial_R(D_1 P) + \partial_R^2(D_2 P)$

$$D_1(R) = \frac{2(d+1)}{d} \text{Wi} R - f(R)R + (d-1)\frac{R_{eq}^2}{R}$$
$$D_2(R) = \frac{2\text{Wi}}{d} + R_{eq}^2$$

Boundary conditions

reflecting at the origin: $-D_1 P + \partial_R(D_2 P) = 0$ at $R = 0$

absorbing at the breakup length: $P(R_{\text{break}}, t) = 0$

Initial condition

monodisperse: $P(R, 0) = \delta(R_0, 0)$

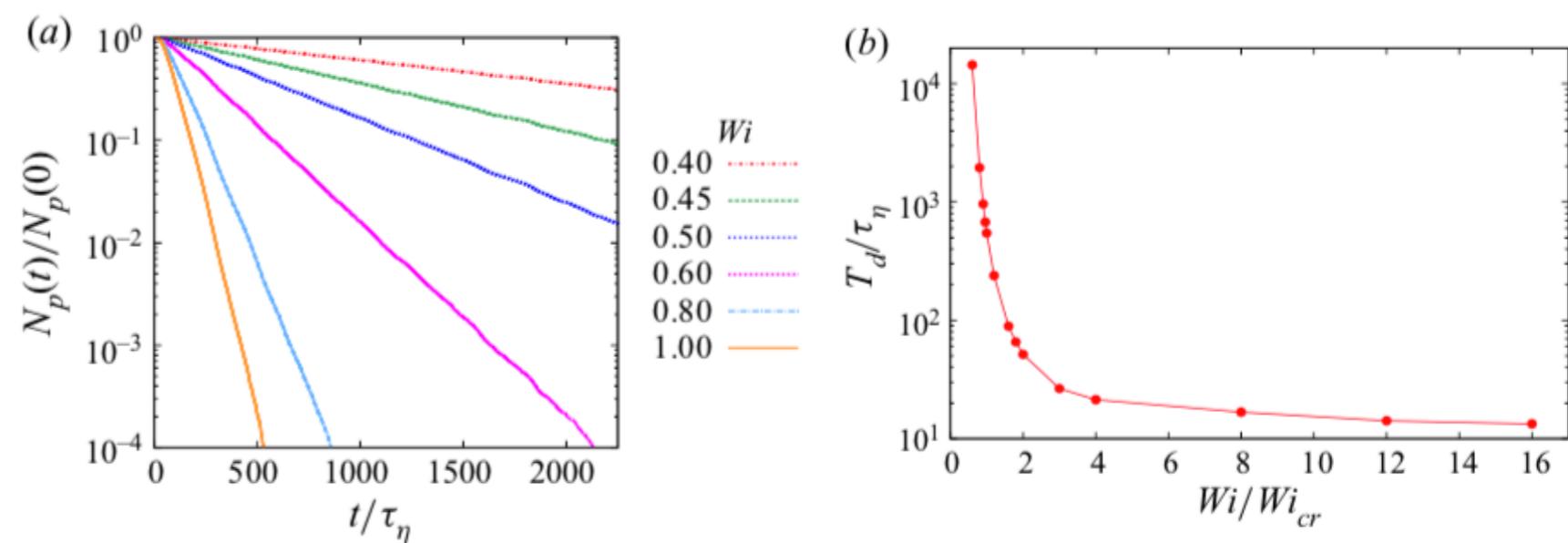
Breakup: Decay of the number of unbroken polymers

Fraction of polymers surviving at time t

$$\frac{N_p(t)}{N_p(0)} = \int_0^{R_{\text{break}}} P(R, t) dt \sim e^{-t/T_d}$$

T_d is the inverse of the smallest positive eigenvalue
of the FP operator with the above b.c.

Lagrangian simulations
in a periodic cube at $R_\lambda \approx 110$
 $N_p(0) = 9 \times 10^5$ polymeric chains
with $\mathcal{N} = 10$ beads each



Breakup: Time integrated PDF of the extension

$$\partial_t P = - \partial_R (D_1 P) + \partial_R^2 (D_2 P)$$

Monodisperse i.e. $P(R,0) = \delta(R_0,0)$

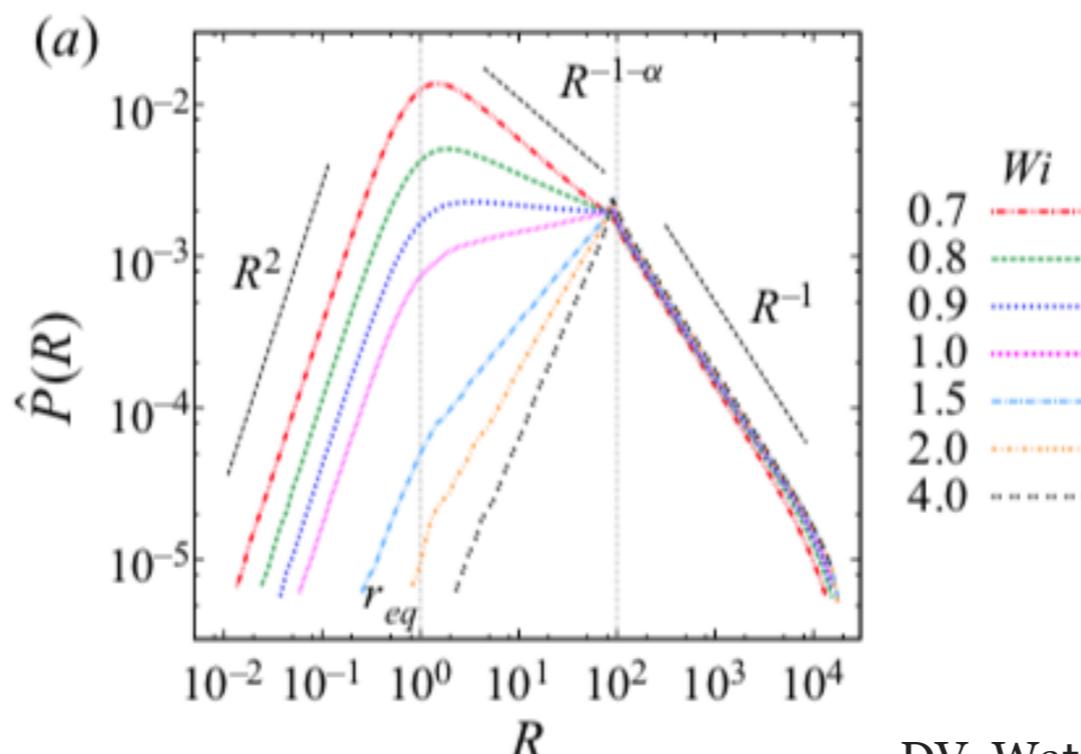
Time integrated PDF of the extension
for unbroken polymers

$$\hat{P}(R) = \int_0^\infty P(R,t) dt$$

$$-D_1 \hat{P} + \frac{d}{dR} (D_2 \hat{P}) = \begin{cases} 1 & \text{if } 0 \leq R \leq R_0 \\ 0 & \text{if } R_0 \leq R \leq R_{\text{break}} \end{cases}$$

$$\hat{P}(R) \sim \begin{cases} R^{d-1} & \text{if } 0 \leq R \leq R_{\text{eq}} \\ R^{-1-\alpha} & \text{if } R_{\text{eq}} \leq R \leq R_0 \\ R^{-1-\beta} & \text{if } R_0 \leq R \leq R_{\text{break}} \end{cases}$$

$$\beta = \begin{cases} \alpha & \text{if } Wi \leq Wi_{\text{cr}} \\ 0 & \text{if } Wi > Wi_{\text{cr}} \end{cases}$$



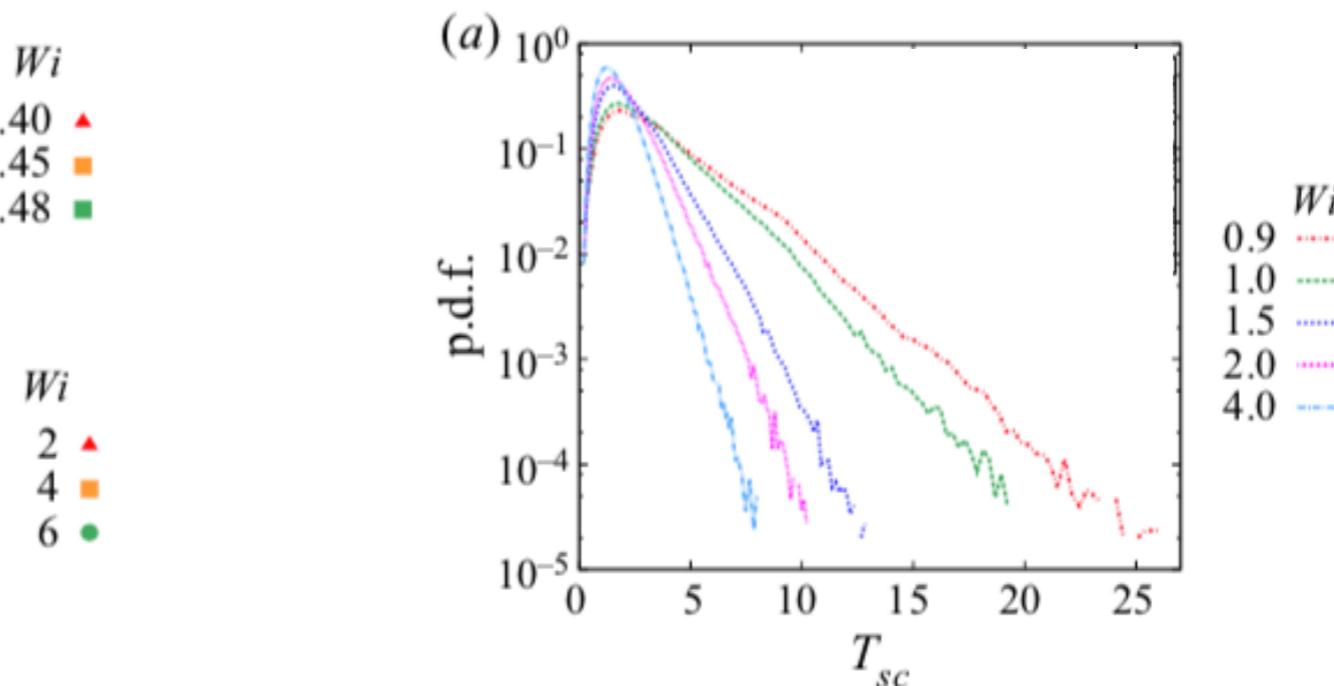
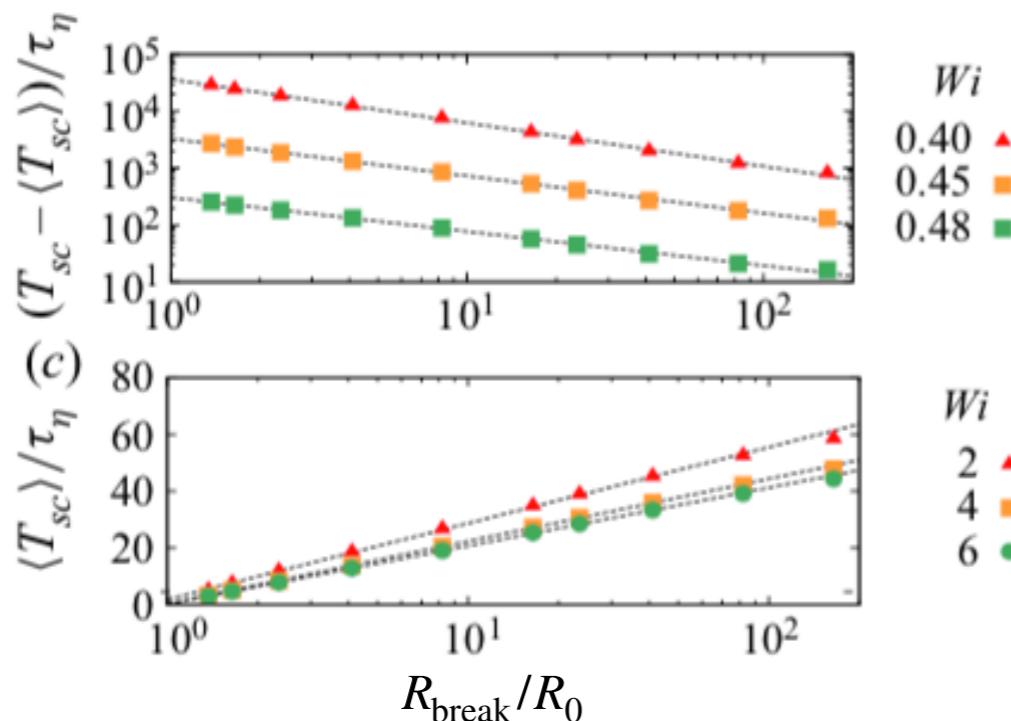
Breakup: Average breakup time

T_{sc} time it takes for a polymer to break in a given realisation of the flow and of thermal noise

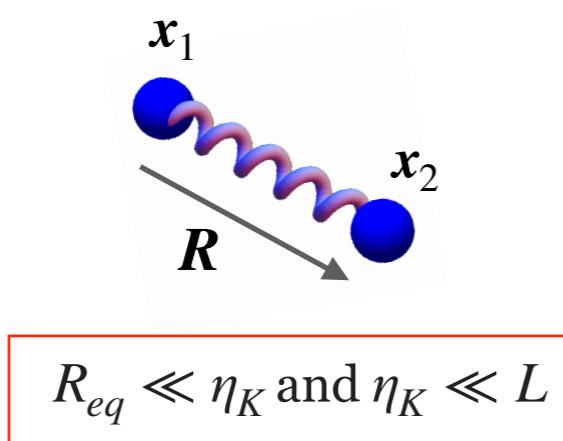
$$F(t) = \text{Prob}\{T_{sc} \geq t\} = \int_0^{R_{\text{break}}} P(R, t) dt$$

$$\langle T_{sc} \rangle = - \int_0^\infty t \partial_t F dt = \int_0^\infty F(t) dt = \int_0^\infty dt \int_0^{R_{\text{break}}} dR P(R, t) = \int_0^{R_{\text{break}}} \hat{P}(R) dR$$

$$\lambda \langle T_{sc} \rangle \sim \begin{cases} \left(\frac{R_{\text{break}}}{R_0} \right)^\beta & \text{if } Wi \leq Wi_{\text{cr}} \\ \ln \left(\frac{R_{\text{break}}}{R_0} \right) & \text{if } Wi > Wi_{\text{cr}} \end{cases}$$



Stretching beyond the Kolmogorov scale

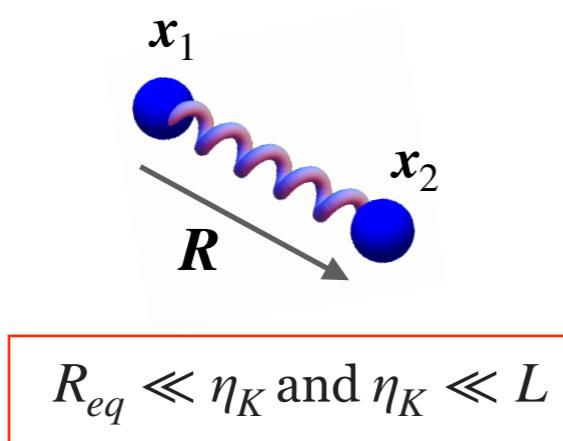


$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \xi(t)$$

$$\frac{d\mathbf{R}}{dt} = \boxed{\mathbf{u}(x_2, t) - \mathbf{u}(x_1, t)} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \xi(t)$$

De Lucia, Mazzino & Vulpiani, *EPL* (2002)
Davoudi & Schumacher, *Phys. Fluids* (2006)

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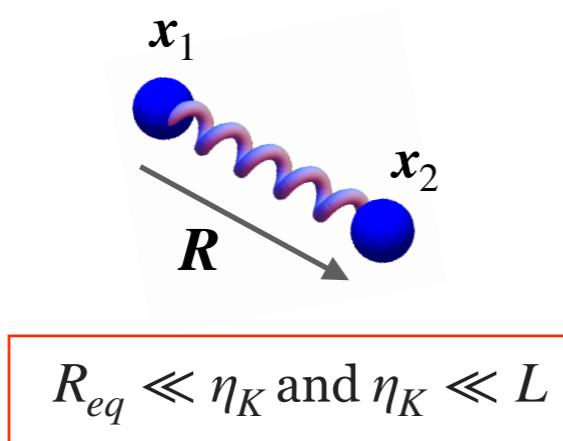
Kraichnan flow

$$\langle u_i(\mathbf{x} + \mathbf{r}, t) u_j(\mathbf{x}, t') \rangle = [D_{ij}(0) - d_{ij}(\mathbf{r})] \delta(t - t')$$

$$d_{ij}(\mathbf{r}) = d_{NN}(r) \delta_{ij} + [d_{LL}(r) - d_{NN}(r)] \hat{r}_i \hat{r}_j$$

$$d_{NN}(r) = d_{LL}(r) + r d'_{LL}(r)/2$$

Stretching beyond the Kolmogorov scale



$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \xi(t)$$

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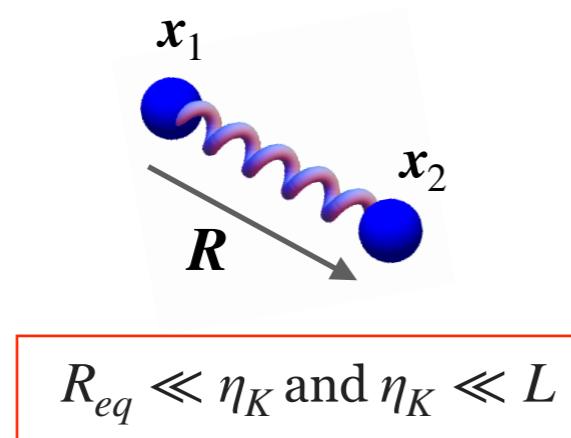
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$$\partial_t P = - \partial_R (D_1 P) + \partial_R^2 (D_2 P)$$

$$\begin{cases} D_1 = \frac{4\tau d_{LL}}{R} + 2\tau d'_{LL} - f(R)R + \frac{2R_0^2}{R} \\ D_2 = 2\tau d_{LL} + R_0^2 \end{cases}$$

Stretching beyond the Kolmogorov scale



$$\frac{d\mathbf{R}}{dt} = \nabla \mathbf{u} \cdot \mathbf{R} - \frac{f(R)}{2\tau} \mathbf{R} + \sqrt{\frac{R_{eq}^2}{\tau}} \xi(t)$$

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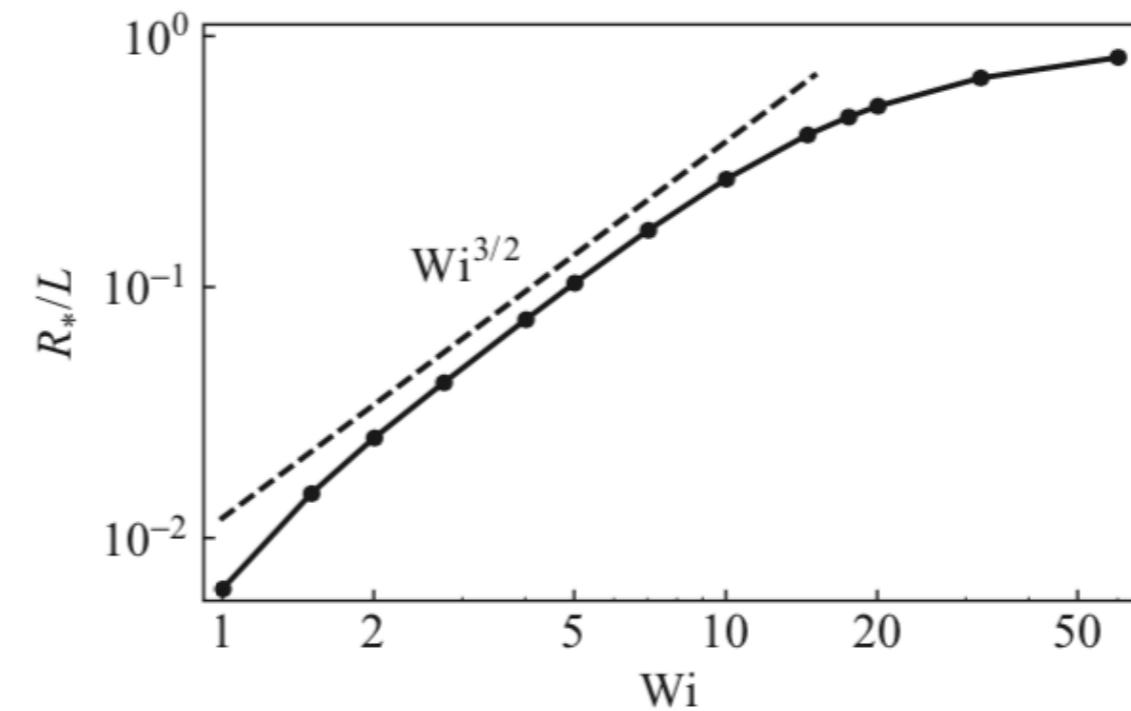
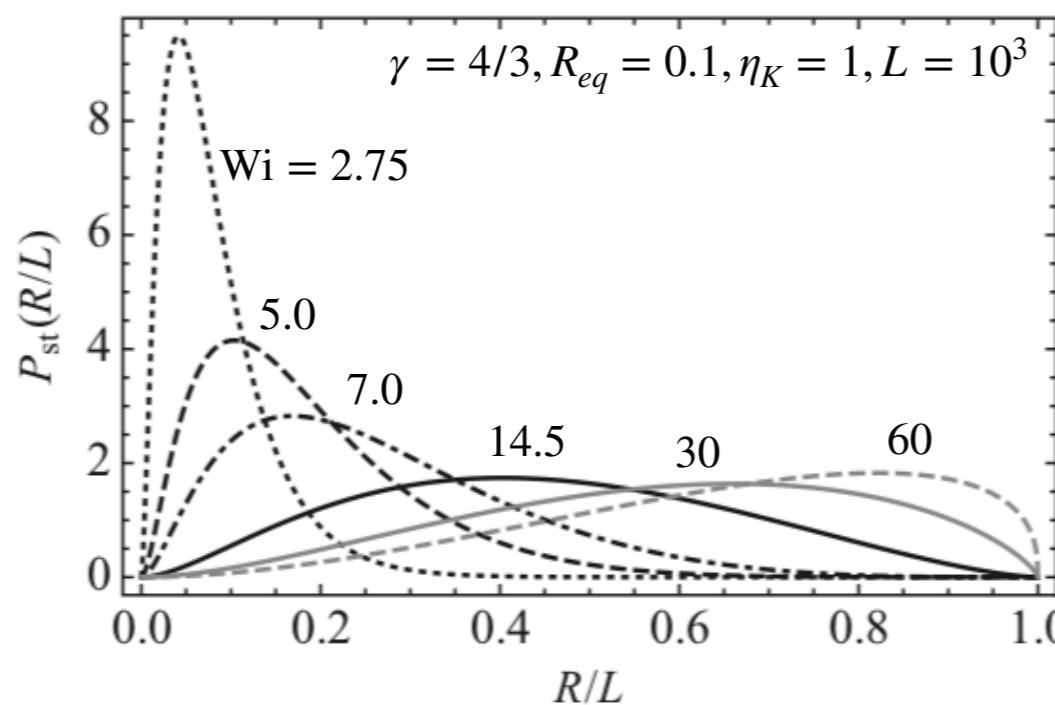
$$E(k) = c e^{-\eta^2 k^2} k^{-1-\gamma} \quad (0 < \gamma < 2)$$

$$\begin{cases} d_{LL} \sim 2D_1 r^2 & (r \ll \eta) \\ d_{LL} \sim 2D_1 a(\gamma) \eta^{2-\gamma} r^\gamma & (r \gg \eta) \end{cases}$$

Stretching beyond the Kolmogorov scale

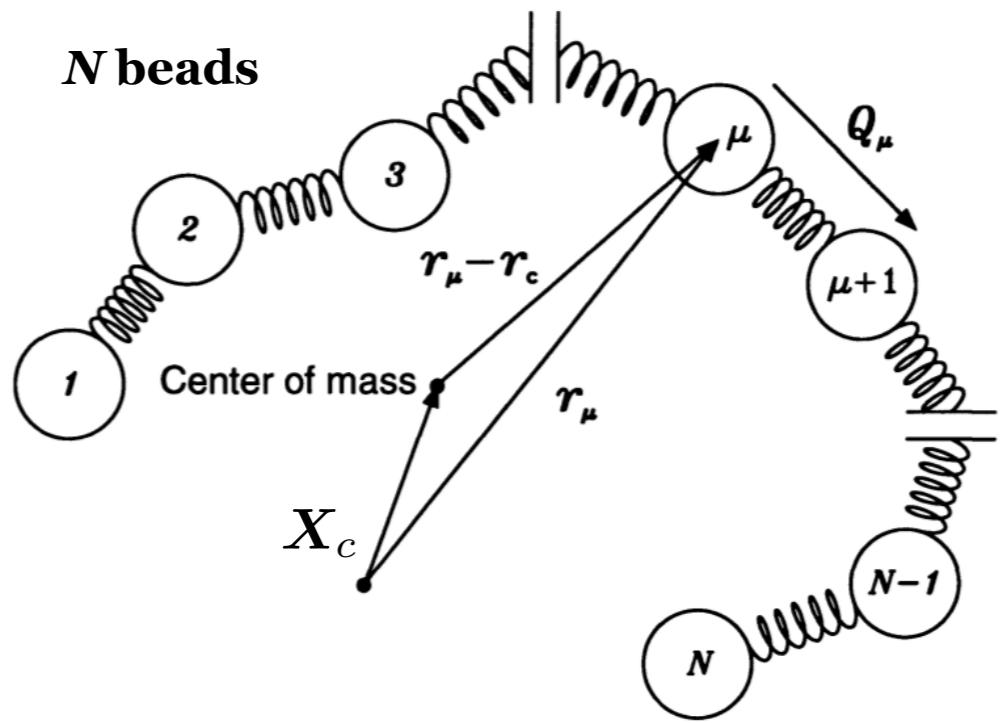
$$P(R) \sim \begin{cases} R^{d-1} & 0 \leq R \ll R_{eq} \\ R^{-1-\alpha} & R_{eq} \ll R \ll \eta_K \\ R^{d-1} \exp\left\{-\frac{a_\gamma}{Wi}\left(\frac{R}{\eta_K}\right)^{2-\gamma}\right\} & \eta_K \ll R \ll L \end{cases}$$

Lumley scale $R_\star \sim \eta_K Wi^{1/(2-\gamma)}$



- The stretched state emerges through the shift of the maximum of the PDF, i.e. R_\star
- There is no coil–stretch transition in this case

Elastic filaments in 2D turbulence



equilibrium length $\ll \ell_f$

$$L_{\max} = (N - 1)Q_{\max} > \ell_f$$

ℓ_f scale of the forcing

$$\frac{dX_c}{dt} = \frac{1}{N} \sum_{i=1}^N \mathbf{u}(x_i, t) + \frac{1}{N} \sqrt{\frac{R_{eq}^2}{6\tau}} \sum_{i=1}^N \boldsymbol{\xi}_i(t)$$

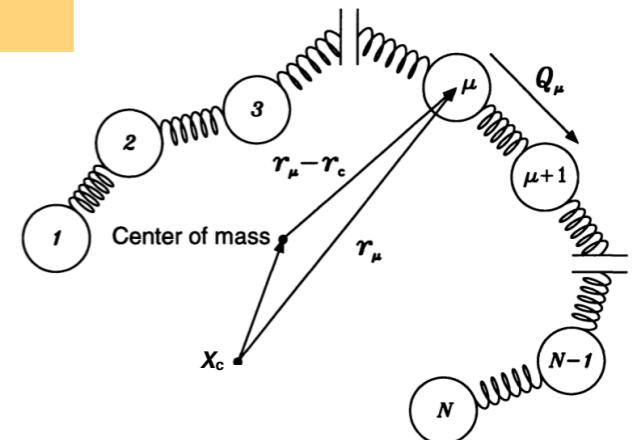
$$\frac{dQ_i}{dt} = \mathbf{u}(x_{i+1}, t) - \mathbf{u}(x_i, t) - \frac{1}{4\tau} (2f_i Q_i - f_{i+1} Q_{i+1} - f_{i-1} Q_{i-1}) + \sqrt{\frac{R_{eq}^2}{6\tau}} [\boldsymbol{\xi}_{i+1}(t) - \boldsymbol{\xi}_i(t)], \quad \tau = 4k/\zeta$$

Preferential sampling of vortices

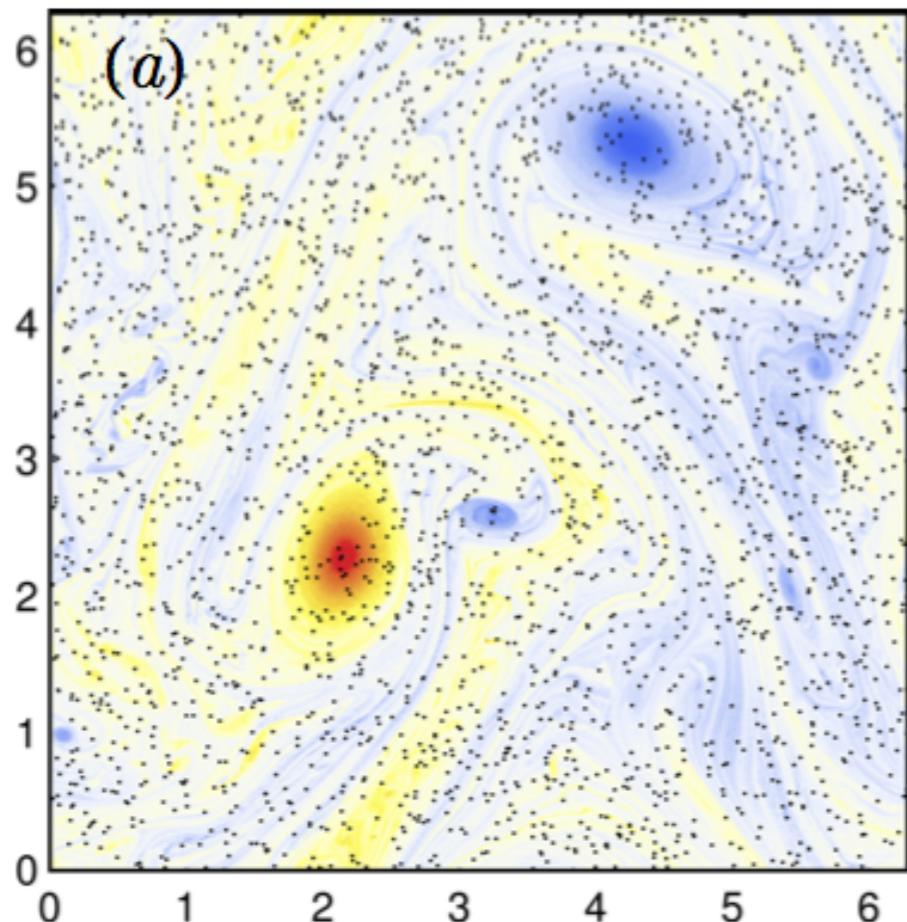
number of beads $N = 10$

chain length $L_{\max} = 4$

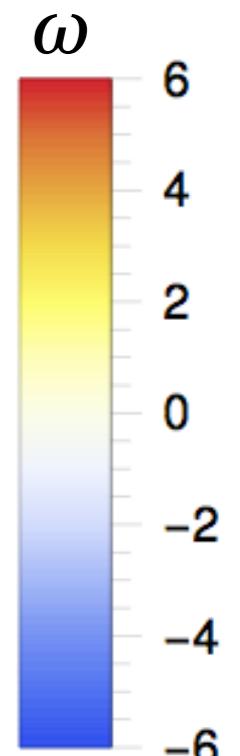
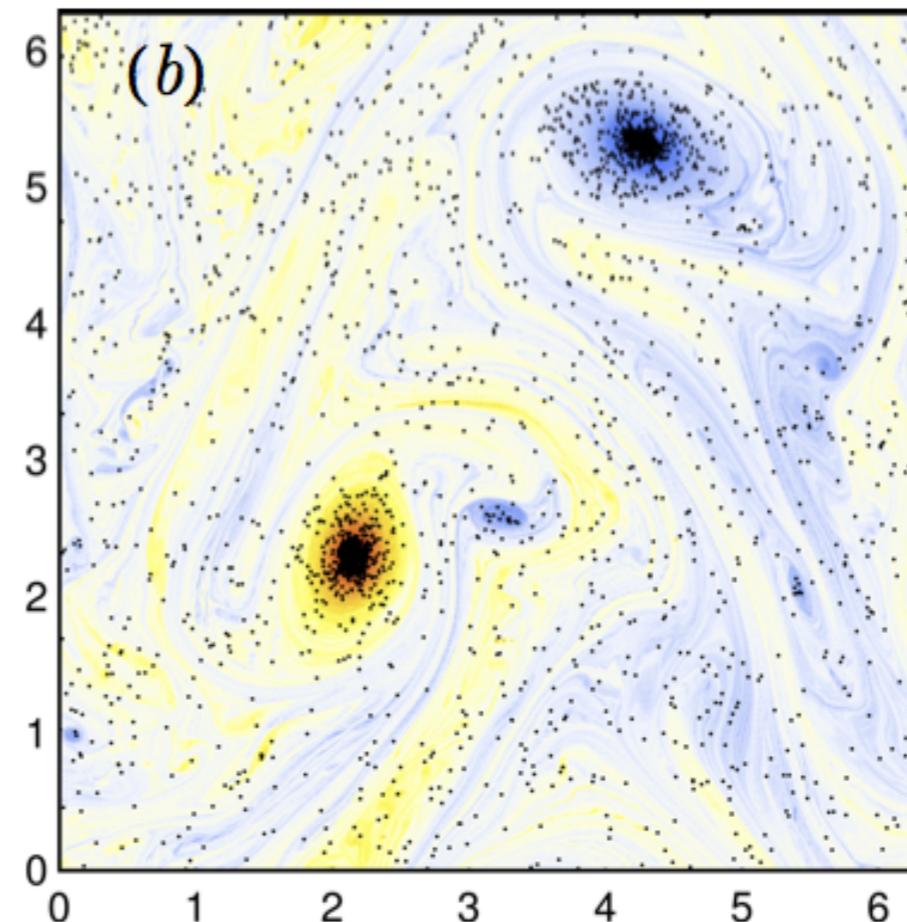
forcing scale $\ell_f = 2\pi/k_f = 2$



Wi = 0.04



Wi = 0.9



Weissenberg number: $Wi = \tau_{\text{chain}}/t_f$ with $t_f = \ell_f/\sqrt{2E}$ (E mean kinetic energy)

2D Navier–Stokes DNS on $[0, 2\pi]^2$, grid resolution 1024^2 , forcing $f = -F_0 k_f \cos(k_f x)$

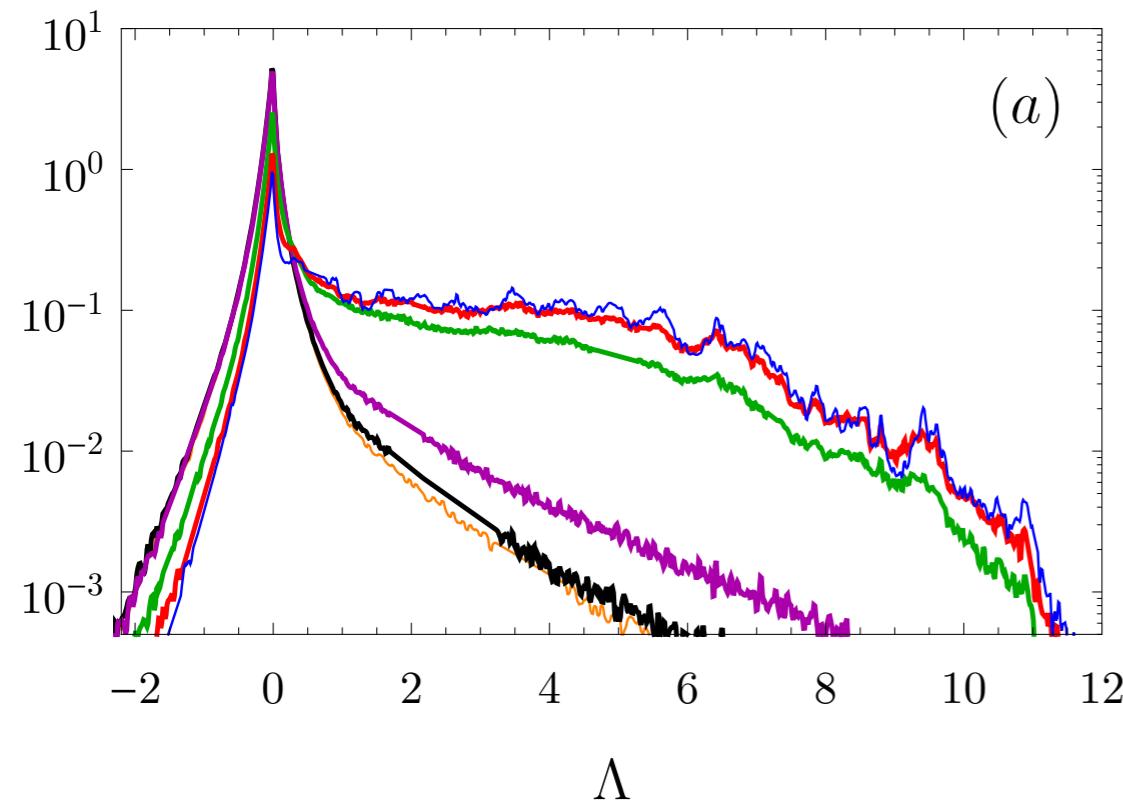
Okubo–Weiss parameter

$$\Lambda = \frac{\omega^2 - \sigma^2}{4\langle\omega^2\rangle}$$

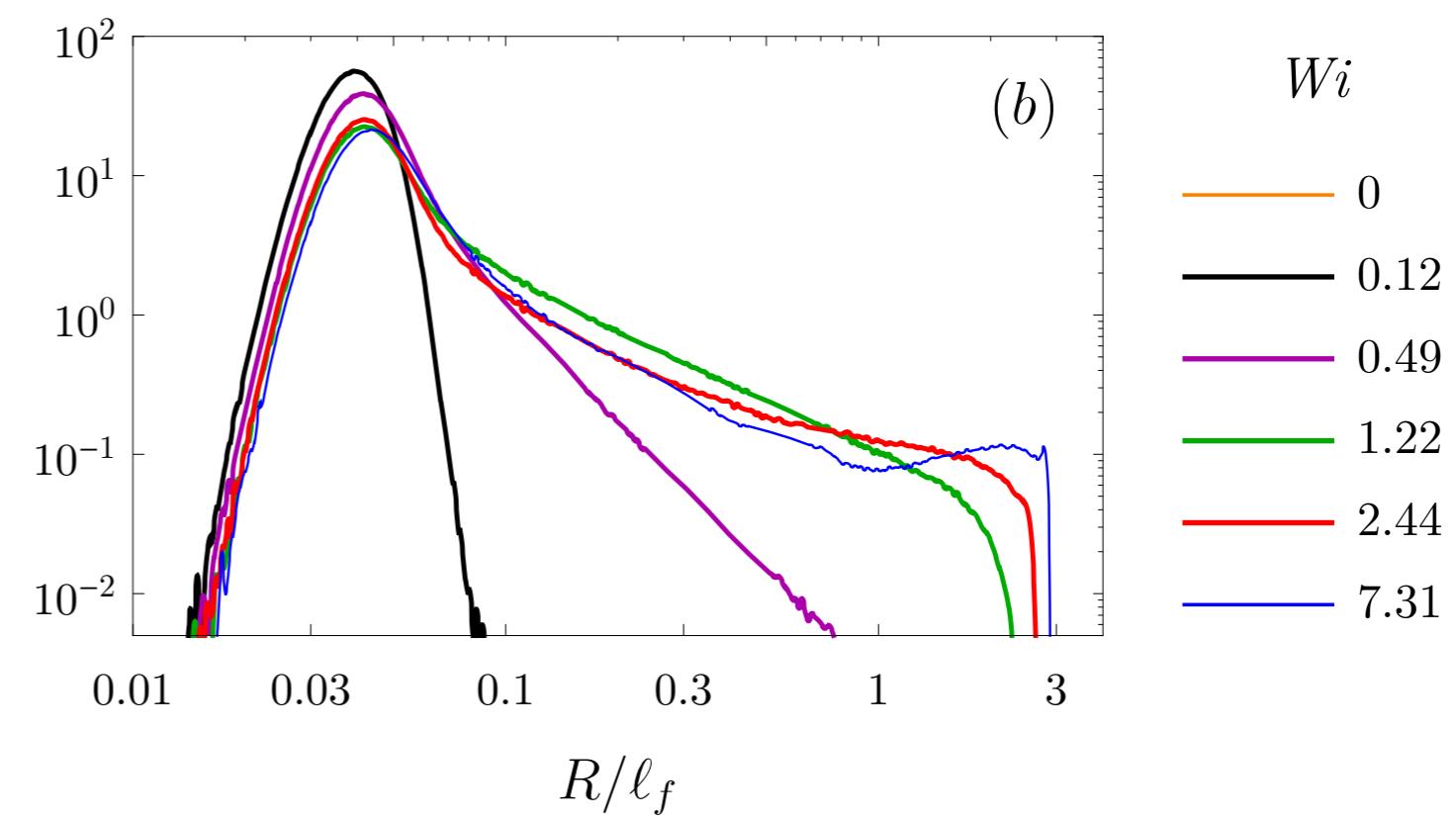
$$\sigma^2 = 2S_{ij}S_{ij} \quad \text{strain rate}$$

$$\mathbf{S} = [\nabla \mathbf{u} + (\nabla \mathbf{u})^\top]/2$$

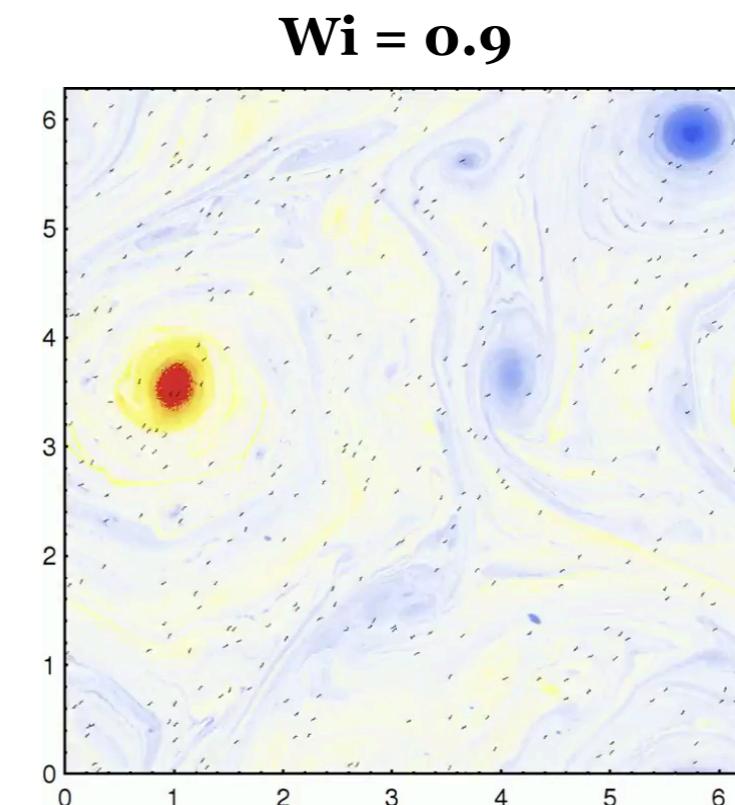
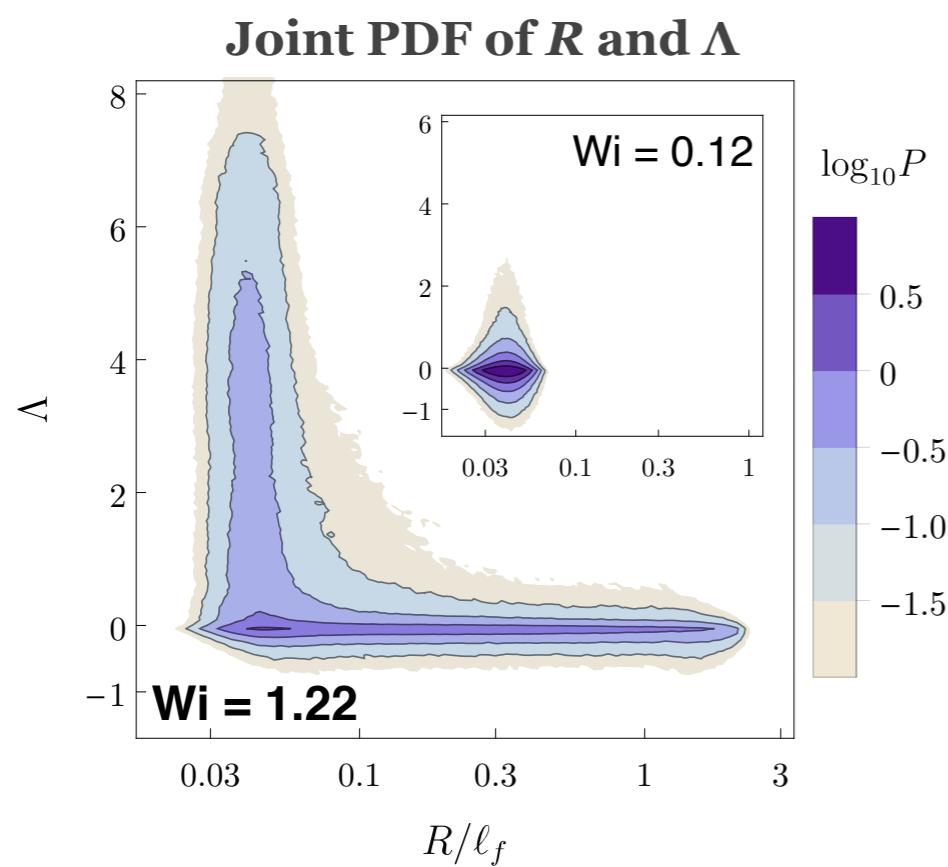
PDF of Λ



PDF of chain extension

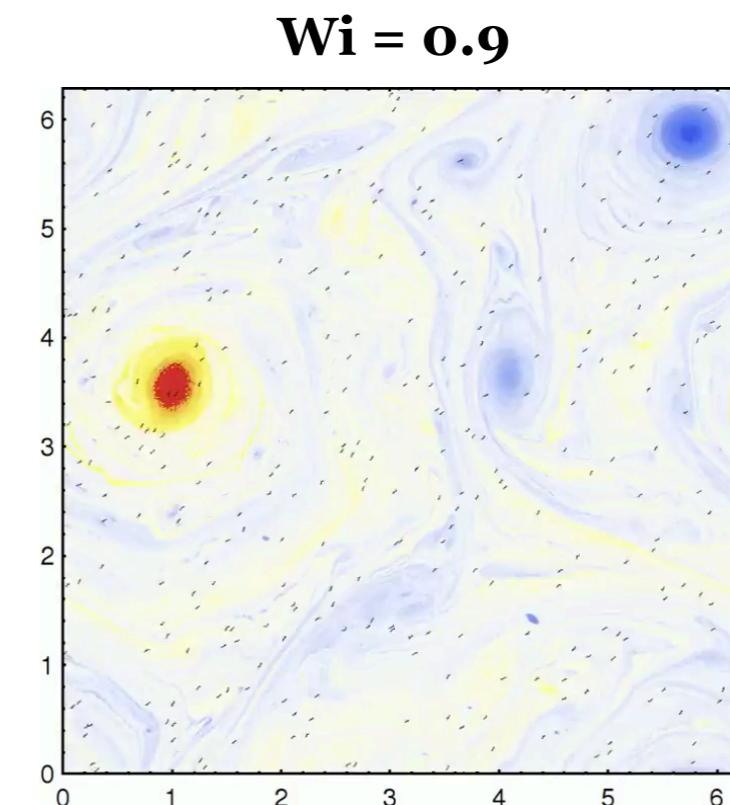
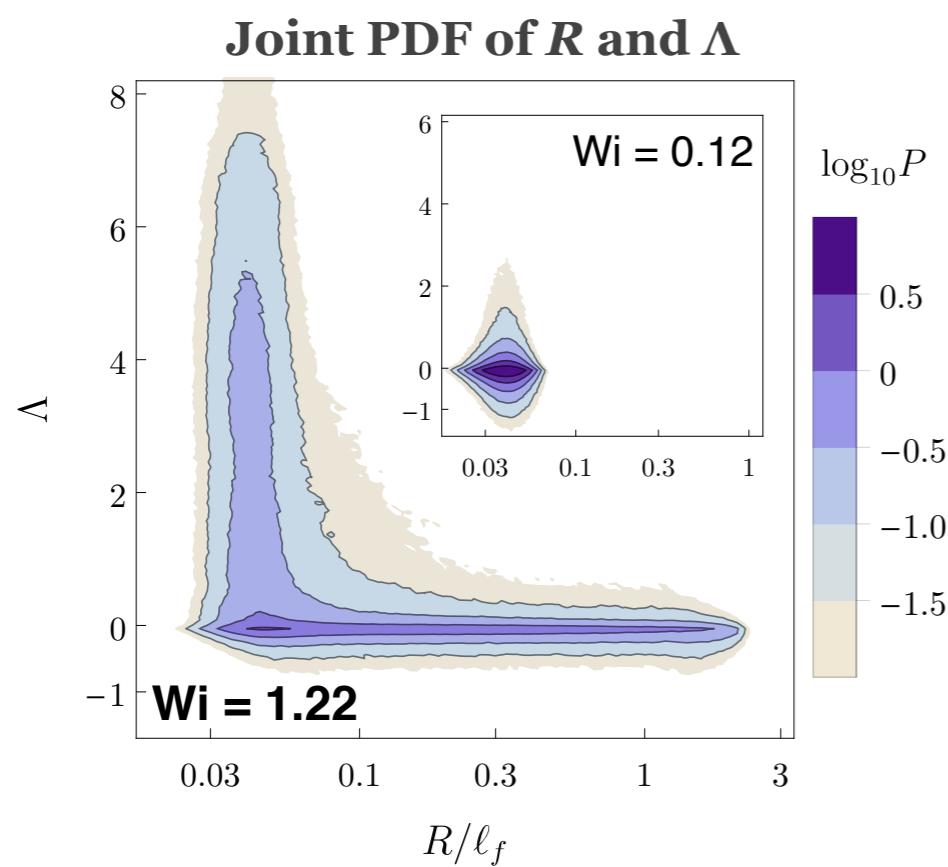


Selection of vortical regions



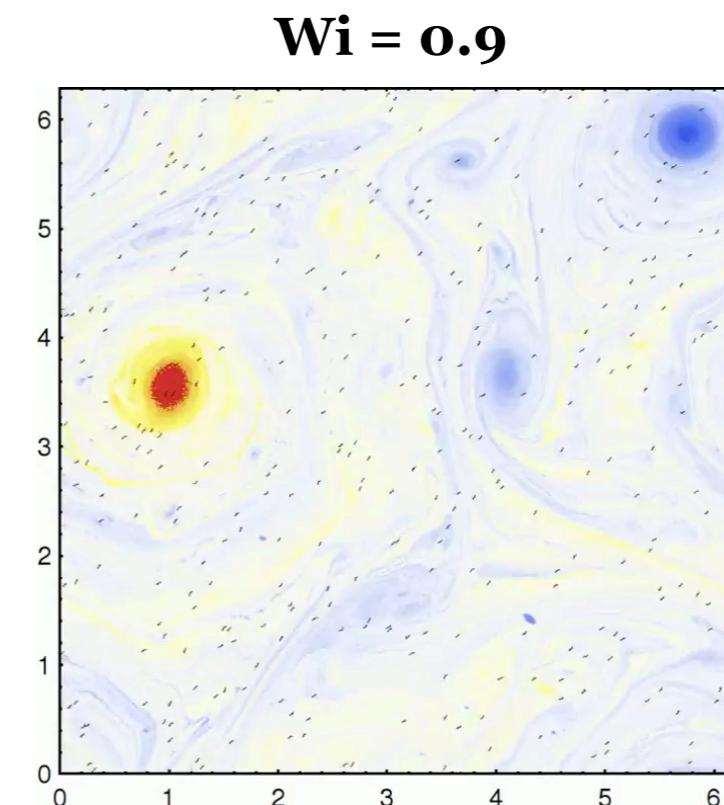
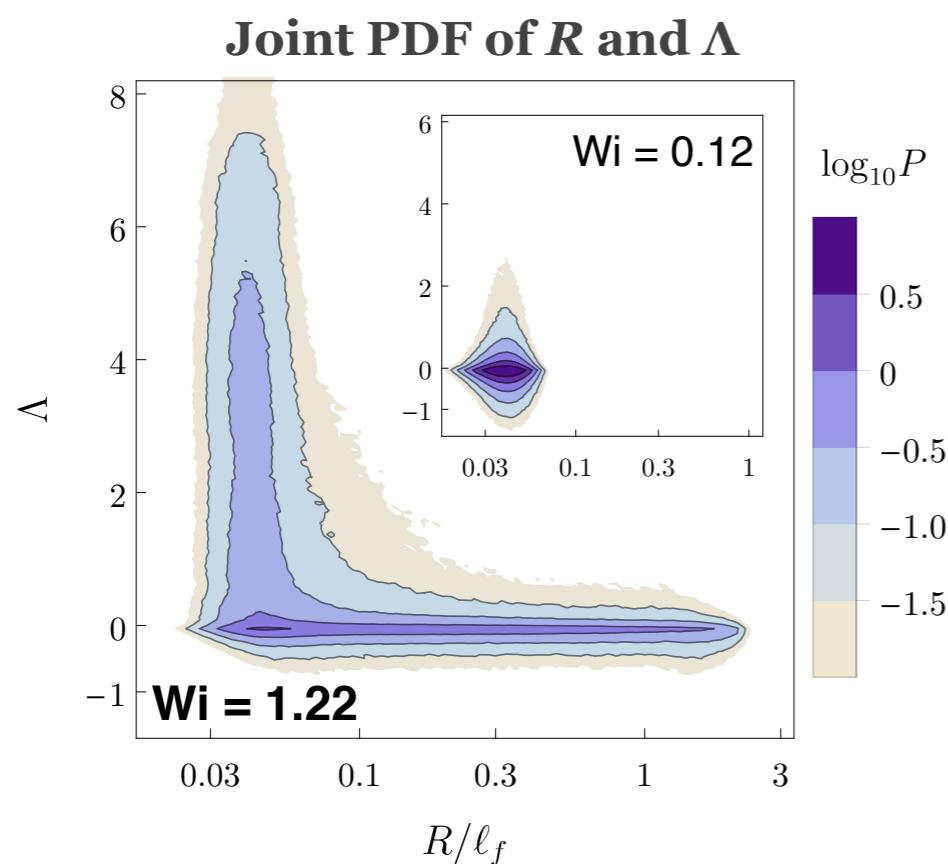
Picardo, DV, Pal & Ray, *Phys. Rev. Lett* (2018)
Singh, Gupta, Picardo, Dv & Ray, *Phys. Rev. E* (2020)
Picardo, Singh, Ray & DV, *Phil. Trans. R. Soc. A* (2020)

Selection of vortical regions



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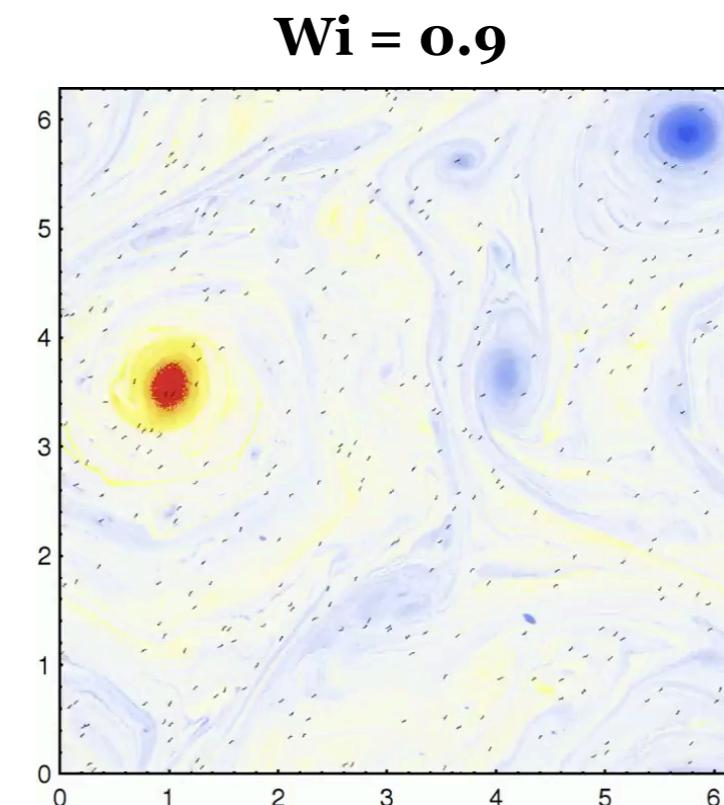
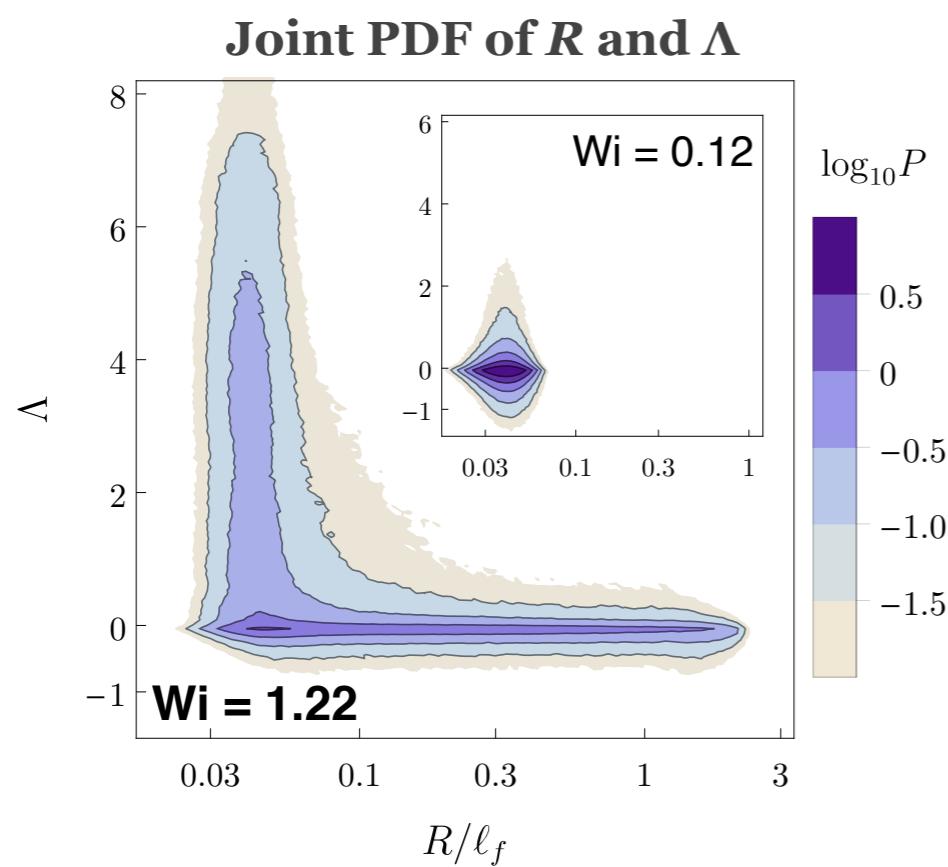
Selection of vortical regions



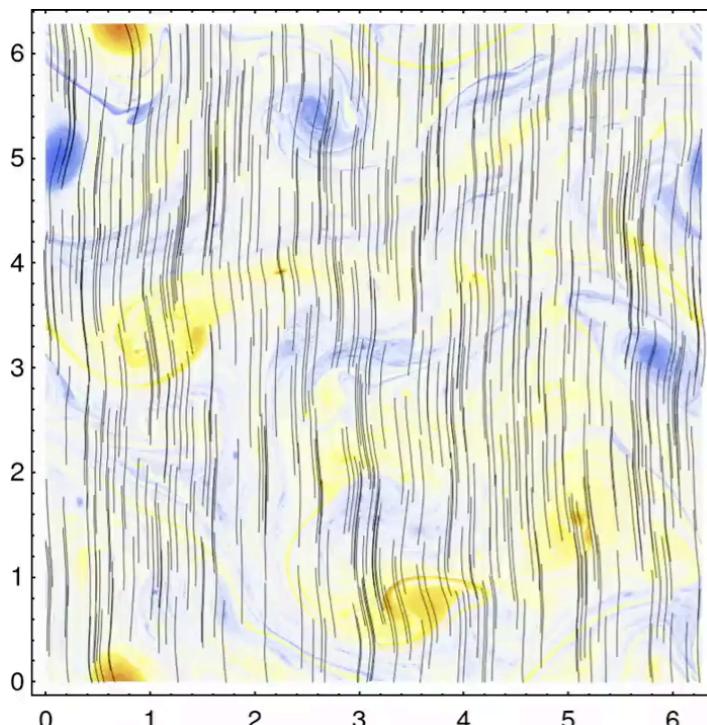
Inextensible filaments

Picardo, DV, Pal & Ray, *Phys. Rev. Lett* (2018)
Singh, Gupta, Picardo, Dv & Ray, *Phys. Rev. E* (2020)
Picardo, Singh, Ray & DV, *Phil. Trans. R. Soc. A* (2020)

Selection of vortical regions

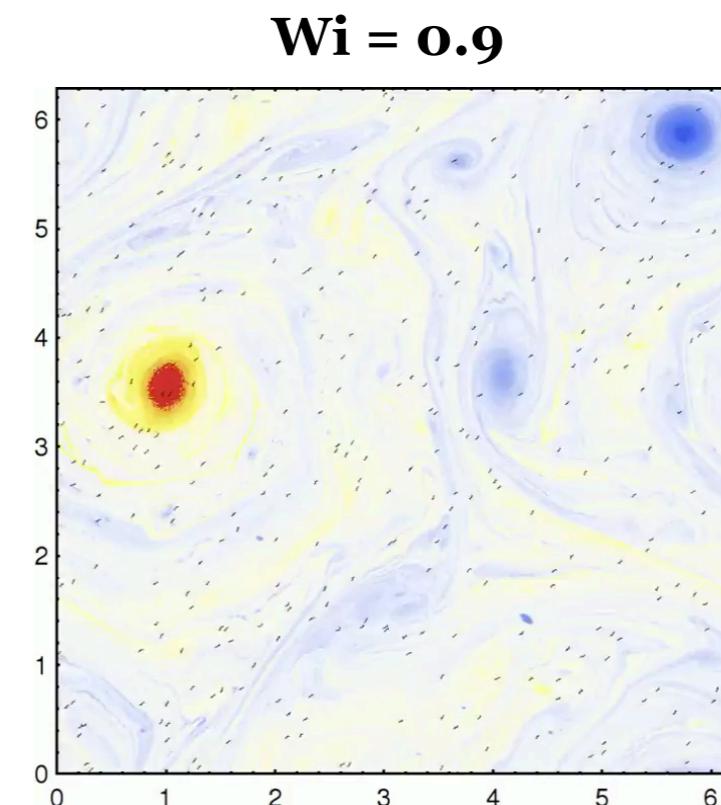
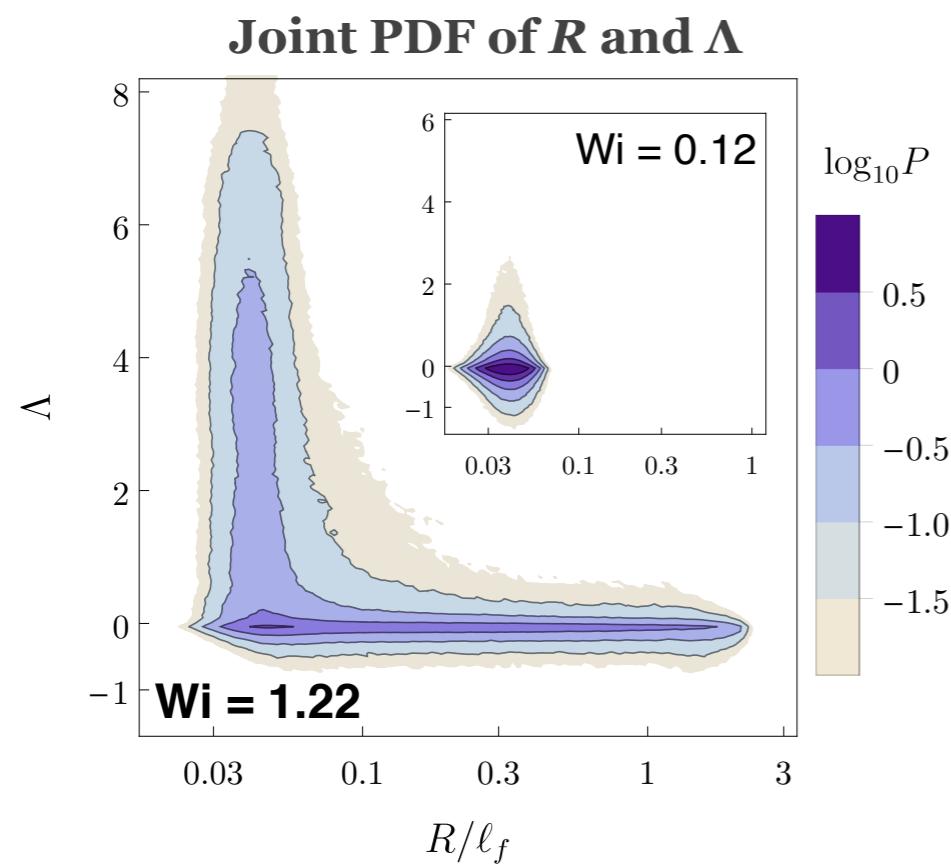


Inextensible filaments

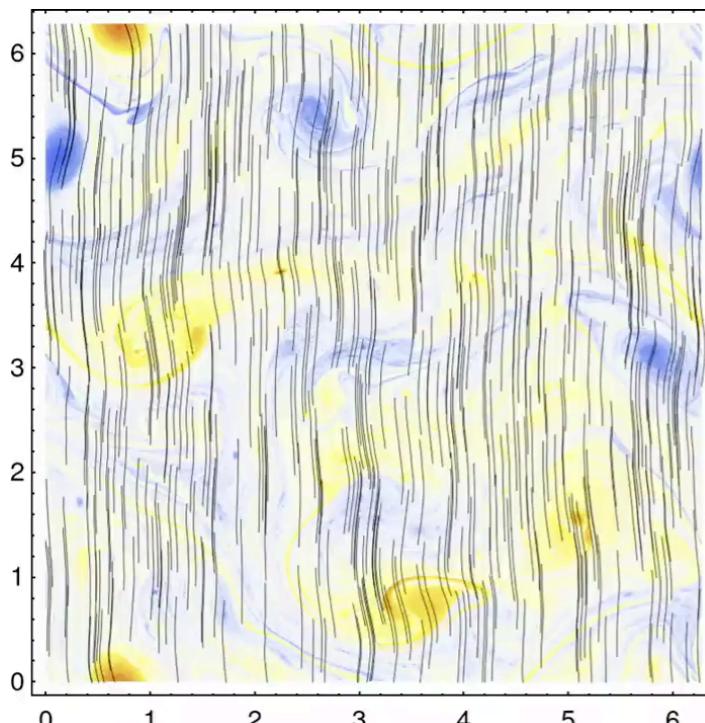


Picardo, DV, Pal & Ray, *Phys. Rev. Lett* (2018)
Singh, Gupta, Picardo, Dv & Ray, *Phys. Rev. E* (2020)
Picardo, Singh, Ray & DV, *Phil. Trans. R. Soc. A* (2020)

Selection of vortical regions



Inextensible filaments



3D turbulence

- The preferential sampling of vortices persists, but is much weaker
- The mechanism is the alignment of the filament with axis of the vortices

Picardo, DV, Pal & Ray, *Phys. Rev. Lett* (2018)
Singh, Gupta, Picardo, Dv & Ray, *Phys. Rev. E* (2020)
Picardo, Singh, Ray & DV, *Phil. Trans. R. Soc. A* (2020)

Perspectives

From *mesoscopic* models of polymer molecules
to *macroscopic* models of polymer solutions:

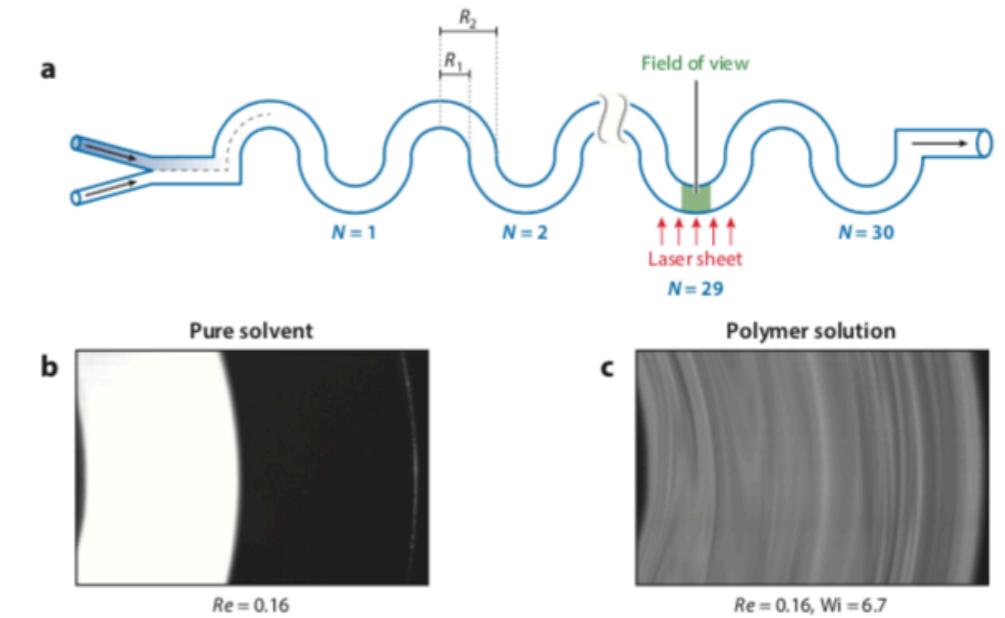
How to include the knowledge on the coil–
stretch transition into continuum models
of polymer solutions?

Turbulent drag reduction (high Re)



White & Mungal, *Annu. Rev. Fluid Mech.* (2008)
Graham, *Phys. Fluids* (2014)

Elastic turbulence (small Re)



Groisman & Steinberg, *Nature* (2000, 2001)
Steinberg, *Annu. Rev. Fluid Mech.* (2021)