Journal of Advances in Science and Technology

Vol. IV, No. VIII, February-2013, ISSN 2230-9659

REVIEW ARTICLE

RELAXATION OF A BEAD-ROD CHAIN

www.ignited.in

Journal of Advances in Science and Technology
Vol. IV, No. VIII, February-2013, ISSN 2230-9659

Relaxation of a Bead-Rod Chain

Sheetal

Research Scholar, CMJ University, Shillong, Meghalaya, India

---------------------------♦-----------------------------

BROWNIAN DESIGN SIMULATIONS ASSOCIATED WITH BEAD-ROD ALONG WITH BEAD-SPRING CHAINS

Quantitative forecasts of the velocity and stretch dispersions in complex streams of polymeric results is a testing objective, however offers the guarantee of additional sane outline of polymer handling operations.

The traditional approach to demonstrating the stream of weaken polymeric results is dependent upon fathoming the comparisons of preservation of mass, force and vigor in conjunction with a shut shape constitutive comparison for the polymeric anxiety. To date, the most regularly utilized shut shape constitutive comparisons for weaken polymeric results have been gotten by approximating models dependent upon dynamic speculation. In any case, such estimates regularly implied as 'closure rough guesses' frequently mutilate the expectations of the definitive dynamic hypothesis based model.

As of late, continuum level discretization strategies have been conclusively combined with Brownian elements (Bd) strategies to permit administer utilization of micro-structural models for polymer motion in stream recreations, consequently by-passing the necessity for shut shape constitutive comparisons. Calculations for effective continuum/mesoscopic re-enactment have propelled at a quick rate since their first introduction in the early 90s. Then again, even with the most productive multi-scale calculations, complex stream re-enactments have been restricted to incorporate just exceptionally basic micro-structural models for the polymeric atom, such as the versatile dumbbell model. This is because of the way that this class of reproductions is extremely Cpu escalated fundamentally because of the vast outfit needed to acquire precise polymeric burdens from Brownian powerful recreations. Subsequently, utilization of additional complex micro-structural models for example bead-rod chains in complex stream re-enactments is past the span of the present figuring force.

To enhance the effectiveness and prescient capacity of joined mesoscopic/continuum reproduction strategies, two issues need to be tended to. First and foremost, more Cpu proficient Bd calculations need to be advanced. Besides, correct coarse-graining systems from a sub-atomic level (i.e. atomistic) to mesoscopic level (e.g. bead-rod and bead-spring chains) need to be created. In what accompanies, we will briskly portray the essential approach in coarse graining from an atomistic to a mesoscopic level of depiction.

The coarse graining from an atomistic level to the bead-rod portrayal is dependent upon sound factual workman standards. Particularly, nuclear vibrations are disregarded accelerating 'freely pivoting bonds'. Also, the separation between the neighboring beads, i.e. the 'kuhn step' could be resolved dependent upon the truth that match smart between nuclear potential face to face times might be dismissed past a certain separation. Further coarse graining from a bead-rod to a bead-spring chain depends on the supposition of neighborhood equilibrated movement of numerous Kuhn steps. Henceforth, various Kuhn steps are reinstated by a 'phantom entropic spring'.

It ought to be noted that hinging on the stream quality, the amount of Kuhn steps that could be comparably reinstated by an entropic spring is diverse; consequently precise coarse-graining strategies from the bead-rod to the bead-spring chains are seldomly accessible. At long last, in the most coarse-grained rough guess, one can disregard the inner structure of the particle and speak for the entire particle as a solitary dumbbell with an entropic spring. Be that as it may, an elective strategy has been proposed by Ghosh et al. who have as of late proposed a coarse-graining strategy dependent upon an adjustable length scale guideline, where the lands of the entropic spring are balanced dependent upon the stream quality.

As specified prior, stream recreations of weaken polymeric results with micromechanical models holding sufficient sub-atomic level informative data to portray the nonlinear rheology of polymeric results, need quick Bd calculations and in addition the requirement for exact coarse-graining systems. Thus, we have centered our consideration on the infrastructure of Cpu effective Bd re-enactment calculations for bead-rod what's more bead-spring chains and in addition the improvement of a discerning coarse-graining system to act for a bead-rod chain by a littler bead-spring chain. Explicitly, we have looked at the exhibition of a completely implied

Newton's system against the normally utilized two-stage mid-indicate system for Bd re-enactment of bead-rod chains. Furthermore, the exactness and Cpu productivity of the stochastically sifted Kramers–kirkwood and the changed Giesekus representations for assessing the polymeric push in bead-rod re-enactments have been analyzed.

Additionally, for the bead-spring models the exhibition of customary express strategies with a completely certain strategy dependent upon Newton's system have been examined. Likewise, two new predictor–corrector based procedures are introduced. Proceeded emphasis of these routines brings about completely self consistent techniques and their exhibition with respect to the other two procedures is talked over. At long last, coarse graining from a bead-rod to a bead-spring chain is examined. The point is to discover the number of Kuhn steps that could be swapped by a proportionate nonlinear entropic spring such that the polymeric stretch figured from both micro-structural models are proportionate over an extensive variety of stream sorts and Weissenberg numbers.

ENERGETIC SIMULATION INVOLVING FREELY-DRAINING, VERSATILE BEAD-ROD CHAINS

The study and advancement of numerical procedures to fathom non-Newtonian liquid mechanics issues has experienced memorable updates lately with the introduction of the Connffessit and Brownian configurational fields strategies which don't require conclusion rough guesses for nonlinear dumbbell models, for example the Fene model. On the other hand, even these routines still include generally straightforward bead-spring models and a set number of modes or springs. The comprehension of the 'physics in the spring' needs further investigation of the weaken result rheology of polymers and is of incredible investment and concern in the literary works. For feeble streams in which the polymer design is just somewhat bothered from the balance design, straight dumbbell models show exceptional concurrence with tests. Trial information for Lagrangian shaky streams with a generous extensional part have been successfully portrayed by means of computations utilizing the nonlinear Fene model yet utilizing physically doubtful Fene parameters. The washout of dumbbell models in solid streams has been ascribeed to an additional thick polymer anxiety which is non attendant in most polymer models.

There have been numerous studies which have recommended models and scalings for gooey polymer pushes in the vicinity of shaky solid streams. Kuhn and Kuhn improved the interior thickness model (Iv model) which elucidates the atomic unbending nature of a polymer and frictional restraints to quick, short length scale mutilations. The interior thickness dumbbell model has a drive following the beads which is corresponding to the rate of miss happening of the spring interfacing the two beads. In spite of the fact that the inside thickness drive is dependent upon atomic notions, the quality can't be promptly evaluated from the sub-atomic structure of the polymer. In the utmost of a limitless inside thickness and numerous bead-springs, the model is comparable to the bead-rod model. Manke and Williams discovered great understanding between the unpredictable thickness of a changed multi bead-Iv model and bead-rod chains. Then again, in extensional stream the multibead-Iv show neglects to expect chain decoding or augmentation which is watched in the bead-rod model. In transient shear stream, the multibead-Iv model predicts impressive motions in the methodology to the enduring state shear consistency and first typical stretch coefficient which have not been watched tentatively. Furthermore, the parceling of the polymer push into flexible and thick segments has not been examined for the multibead-Iv model.

Most other models of viscous stresses for flexible polymers have used rigidly constrained beads which result in viscous stresses (in addition to the usual Brownian stresses) analogous to that in a rigid rod suspension. Acierno et al. were among the first to use a non-Brownian bead-rod model to develop a physical basis for viscous polymer stresses in extensional flow. King and James later suggested a frozen-necklace model in which a Rouse chain in extensional flow becomes frozen into a fixed configuration. In both the bead-rod and frozen-necklace models the viscous polymer stress is due to the rigid constraints imposed on the polymer motion. Rallison and Hinch showed the large viscous stresses for non-Brownian bead-rod chains in extensional flow are due to backloops which form during the unravelling of the chain. Guided by the backloop concept, Larson developed a novel kink dynamics model in which a polymer unravels like a one dimensional non-Brownian string and viscous forces arise due to the inextensibility of the string. Hinch performed both Brownian and non-Brownian simulations of bead-rod chains along with the kink-dynamics model and concluded that the polymer stress in strong flows is mostly viscous. The viscous polymer stress was found to scale with R_g^4/N where R_g is the chain radius of gyration and *N* is the number of beads. His simulation method for the Brownian chains was not rigorous and was later modified to study the relaxation of bead-rod chains from an initially unraveled configuration. Thus these previous bead-rod studies fail to unambiguously determine the relative magnitudes of the viscous and the elastic polymer stresses.

Formerly we improved an intends to divide the flexible and gooey commitment to the polymer push for Kramers' bead-rod chains. In consistent shear and extensional stream we discovered that the anxiety is commanded by the versatile segment for all sensible Wi where the Wi is the product of the shear (or amplification) rate and the longest unwinding time of the chain.

In extensional stream, the thick stretch comes to be as hefty as the flexible at $Wi=0.06n^2$. As of late, Rallison has numerically affirmed the consistent state stretch parceling for minor chains $(N \leq 10)$ in planar extensional stream however in his estimations for the begin up of elongational stream he utilized a bead-firm-spring model and subsequently was unable to process a thick polymer anxiety.

For Rallison's begin up reproductions he presumed that a huge thick polymer anxiety exists in transient streams which scales with R_g^2. This conclusion is dependent upon how the polymer anxiety scales with the span of gyration tensor and not by verifying the genuine dividing of the polymer hassles. He does prescribe the stretch that he terms as "thick" may really be a versatile stretch with a quick unwinding time. In the present study, we utilize our re-enactment system and unambiguously confirm the parceling of the burdens in transient streams for bead-rod chains.

The bead-rod chain is a coarse grain model of an atomistic polymer chain however is still as well awkward for the numerical result of most non-Newtonian liquid mechanics issues. Rather basic bead-spring models are regularly utilized. The definitive advancement of the spring drive in these models is dependent upon the entropic restoring compel for a bead-rod chain.

The power needed to expand the chain end-to-end partition is straight at long last to-end partition for minor distortions and is given by the reverse Langevin capacity for expansive mutilations. The Hookean spring compel compares to the straight cutoff and the FENE spring energy is a numerical estimate of the nonlinear point of confinement. There is hence an immediate relationship between the spring constants and the bead-rod chain parameters. These models could be altered to incorporate numerous beads associated continuously by springs (Rouse and multibead FENE models). The polymer stretch in the FENE and Rouse model is immaculately versatile on the grounds that the spring power law is inferred from entropic restoring compels. The Rouse model founders in solid streams unpaid to an unbound development of the chain microstructure. Examinations of the FENE model to test information have for the most part made utilization of the Peterlin close estimation to pre average the nonlinear FENE constrain, normally implied as the FENE-P model. Modest qualities for the greatest extensibility of the dumbbell were demanded to get quantitative concurrence with investigations. While it is clear that the limited extensibility of the FENE dumbbell is physically sensible, the greatness of the nonlinear flexible anxieties in solid streams and the best possible way to pick the greatest extensibility of the dumbbell is not clear. An alternate test of the FENE model is an observation to the more entangled bead-rod demonstrate from which it was basically determined. Formerly, we exhibited that FENE dumbbells are in great assention with the consistent state shear and elongational rheology of bead-rod chains, however we didn't figure transient lands of either model.

Tentatively one can measure polymer hassles utilizing birefringence if the anxiety optic law is quality. Examinations have affirmed the legitimacy of the anxiety optic law for powerless shear stream, while under solid stream conditions the anxiety optic law is not for the most part good. Smyth et al. have affirmed the being of thick burdens for semi dilute results of semi rigid polymers in enduring shear stream and have indicated that the anxiety optic law is good for the versatile part of the polymer anxiety. A captivating set of fiber extending analyses utilizing Boger liquids have as of late been performed by Spiegelberg and Mckinley in which the anxiety optic law throughout the beginning of extensional stream was good up to a certain strain. It is not as of now known if the inadequacy of the anxiety optic law for adaptable polymer results in solid streams is because of an extra polymer thick push or a nonlinear versatile polymer anxiety. Figuring out this won't just help in the key comprehension of polymer anxieties in solid streams yet is the first stage in advancing a changed push optic relationship for profoundly enlarged weaken polymers.

In this study we put forth comes about for the transient hassles and birefringence of weaken bead-rod chains in shear and uniaxial elongational stream. We think about three primary focuses: apportioning of the anxieties into gooey and flexible parts, correlation to the FENE dumbbell, Animate chains and FENE-PM model and the quality of the anxiety optic law. Begin up of uniaxial extensional and shear stream is put forth for an extensive variety of Wi and N. The polymer anxiety is divided into its gooey and flexible parts and we figure out the time scale and Flow quality over which the thick commitment is critical. We confirm when and why the stress-optic law starts to fall flat. The reproduction comes about for the bead-rod chains are contrasted with Brownian elements reproductions of FENE dumbbells, numerical counts of a multimode Animate chain and a multimode FENE-PM chain. A basic appraisal is made of the bead spring models and if their inadequacies are made by pre averaging close estimations, coarse graining, or more basic physical issues. The extensional consistency expected by the FENE and FENE-PM models is contrasted with trial information of weaken polystyrene solutions.

CONFORMATIONAL RELAXATION OF AN IN THE BEGINNING IS TRAIGHT HARD BEAD-ROD POLYMER

The present study acknowledges the relaxation of a solitary solid polymer chain from a starting straight arrangement in a viscous dissolvable. Physically this issue may compare to the instance of a polymer chain completely extended by an in number stream and after that loose by switching the stream off. This issue is additionally persuaded by later explores different avenues regarding single living molecules unwinding in the wake of being completely augmented by connected drives and in addition by the later advancement of micro devices involving extended tethered biopolymers. In this article, we center our consideration on the anxiety and birefringence relaxation and how they are influenced by the relating design relaxation. Our investment falsehoods on solid polymers—i.e., polymers whose ingenuity length is bigger than their form length. Our effects are appropriate to both engineered and living hardened polymers for example Kevlar. polyesters, actin fibers, microtubules and rodlike infections.

The investigation of the progress of semi flexible polymers has appropriated much consideration throughout the final years. The persistence length of distinctive particles of these polymers shifts from 50 nm for Dna to close to 15 /xm for F-actin and 10 mm for microtubules. By recognizing that the littlest length connected with these biopolymers is the diameter of the single particle with an average worth of a couple of nanometers, we promptly acknowledge that semi flexible polymers demonstrate a wide run of solidness which brings about some extraordinary lands of their results and systems. Therefore, there has been as of late a developing premium in comprehension the lands of semiflexible polymers by both exploratory and speculative examinations.

Test studies utilizing macro rheological and micro rheological methodologies have recognized the viscoelas-ticity of Faction results and systems, microtubules, and engineered polymers. Single-particle examining procedures have permitted the examination of the flow of Dna atoms and stiffer natural polymers for example action fibers and microtubules. Speculative investigations recognized both the compliance and viscoelasticity of semi flexible polymer results particularly close harmony. Investigations of polymer results far from equilibrium incorporate the issue of the chain being straightened by connected drives and also the motion of a chain under different outer irritations.

In this study we examine the anxiety and birefringence relaxation of an at first straight solid polymer. Various authors have examined the comparing issue for adaptable polymers. Although we unequivocally recognize the relaxation of a solitary polymer chain in a thick dissolvable, our effects ought to be quality indeed, for thought polymer results and arranges with the expectation that the relaxation of investment happens on length scales shorter than that portraying the traps or crosslinks.

DYNAMICS AND THE EFFECTS OF HYDRODYNAMIC INTERACTIONS

The ability to directly visualize individual DNA molecules via fluorescent staining allows one to obtain experimental data on the behavior of individual polymer molecules.[1-8] Recent work[9,11] has shown that simple bead- spring or bead-rod models can reproduce some of the non- equilibrium properties of λ-phage DNA. That work has also demonstrated that, provided the friction coefficient is determined from the experimental relaxation time, these simple models can reproduce some properties of nondilute solutions.[11] As important as that work has been, the models employed in these references have not included excluded volume effects or hydrodynamic interactions, and therefore cannot be used as predictive tools for molecules of differing sizes. Furthermore, experimental evidence" indicates non-free-draining behavior for DNA molecules as short as 3 μm. Recent studies[12-14] have considered both excluded volume and hydrodynamic interactions in stochastic simulations of DNA. However, that work only considered chains of less than a micron in length and simulation times of less than a second. For simulations of transport in microfluidic devices which involve external fields, such as those proposed for DNA separation. A sound treatment of hydrodynamic interactions is essential.

In this work we present a fully parametrized bead-spring model for DNA which includes finite extensibility, excluded volume effects and hydrodynamic interactions. The parameters in the model are inferred from available experimental data for 21 μm λ-phage DNA. The model satisfies all the molecular weight scaling laws for dilute solutions of linear polymers, and therefore is expected to provide a useful predictive tool at higher molecular weights.

EFFECT OF HYDRODYNAMIC INTERACTIONS ON DNA DYNAMICS IN EXTENSIONAL FLOW

The non equilibrium conduct of adaptable polymer particles in streams of weaken results is mind boggling, and a correct portrayal of the motion of long-chain macromolecules could be an overwhelming assignment. Customarily, mass rheological tests incorporating stream birefringence and light dispersing estimations were utilized to surmise informative data observing polymer conformation, introduction, and chain extend in solid streams. All the more as of late, the coming of single particle visualizations utilizing fluorescence microscopy has considered the straight perception of single Dna atoms in streams of weaken results in shear, planar extensional, and general two-dimensional blended streams. Trial comes about because of these studies have illustrated complex polymer conduct in various ways. First and foremost, investigations of Dna take into account perception of generally portrayed, mono-scatter polymer chains of known form length, with balance lands for example chain diffusivity and polymer relaxation times known inside small degrees of exploratory doubt. Besides, perception of transient atomic stretch uncovers rich individualistic atomic conduct concerning chain configuration. Weaken result studies including Dna are performed at to a great degree flat fixations ($\approx 10^{-5}c^*$, where c* is the polymer cover focus) such that inter polymer collaborations are missing and make no stream affected progressions an overall demarcated, spatially homogeneous stream field. Results incorporating transient and consistent chain extend in stream have considered noteworthy advancement to be made in zones of model advancement and recreation calculation testing. Model parameters may be picked such that the reproduction exactly catches known lands of Dna particles, and the non equilibrium micro structual qualified information between investigation and reproduction may be straight thought about. A cautious coupling of single atom visualization and Brownian elements re-enactment of polymer chains furnishes an effective blending of instruments to study the elements of polymer chains in stream.

Numerous past Brownian progress recreations of bead-spring and bead-rod models for lambda Dna chains have incorporated the presumption that polymer chains are free-emptying, though the creators calculate bead drag coefficients to match the longest polymer relaxtion time measured from analysis. As talked over beneath, such models for lambda Dna show quantitative concurrence with dynamical polymer conduct determined from single particle investigations. In a free-emptying bead-spring polymer model, the sum of the beads travel through the dissolvable without affecting perturbations to the dissolvable velocity. Notwithstanding, in a practical polymer chain, partitions of the polymer irritate the dissolvable stream field, and close-by districts of the particle are influenced by these hydrodynamic connections (Hi). In the curled state, inner part monomer units are shielded from the full dissolvable velocity by external partitions of the atom. Notwithstanding, in the completely augmented adaptation, monomer units are more presented to the stream, and the impacts of Hi are reduced. In this state, the liquid pushes a more viable frictional grasp on the polymer atom.

Hydrodynamic interactions have well-known effects on the linear viscoelastic (LVE) properties of polymers. The longest polymer relaxtion time r scales as molecular weight M like $\tau \sim M^{1.5}$ for HI-dominant polymers in a 0 solvent and $\tau \sim M^{1.8}$ for polymer chains in a good solvent, compared to $\tau \sim M^{2}$ for free-draining chains. Furthermore, the storage and loss moduli from oscillator}' LVE measurements scale with frequency ω as $\omega^{2/3}$ rather than $\omega^{1/2}$ in the intermediate frequency regime for polymers in solvents. As pointed out by Hsieh et al., inclusion of HI is required even for an accurate qualitative description of the linear rheological behavior of dilute solutions of macromolecules.

Notwithstanding Brownian motion (Bd) reproduction of free-emptying polymer models, some later studies have additionally concentrated on the impacts of intrachain Hi and rejected volume on polymer motion in extensional stream. Cifre and de la Torre examined the weaken result conduct of adaptable polymers in relentless uniaxial extensional stream utilizing Bd reproduction of bead-spring chains with Hi and prohibited volume (Ev) face to face times. In a supplemental study, Cifre and de la Torre explored the rate of polymer curl unwinding in transient extensional streams utilizing Bd recreation of bead-spring chains with Hi and Ev. Utilizing a bead-rod demonstrate with intramolecular Hi and Ev, Neelov et al. re-enacted the conduct of straight polymers in extensional stream utilizing Bd reproduction. In this live up to expectations, the creators deter¬mine a sub-atomic weight scaling for the basic extensional stream rate at which the atoms show the curl extend move in extensional stream. Neelov and Adolf enlarged this unique work for direct polymers to dendrimers in uniaxial extensional stream, again utilizing a bead-rod show with intramolecular Hi and avoided volume collaborations.

The effects of HI on the nonequilibrium dynamics of polymer molecules have been previously studied using kinetic theory. Zimm represented bead disturbances to the solvent flow field as point forces (Stokeslets). For viscous dominated (low Reynolds number) flows, a velocity disturbance $\mathbf{v}'(\mathbf{r}')$ at a location $\mathbf{r}'$ is linearly proportional to the disturbance force F that a neighboring bead at location r exerts on the solvent, giving $\mathbf{v}'(\mathbf{r}') = \mathbf{G}\cdot\mathbf{F}(\mathbf{r})$, where G is the Green's function of the time-independent, linear Navier—Stokes equation. Inclusion of these interactions into polymer kinetic theory yields nonlinear equations for the moments of the polymer end-to-end vector, even for chains with a linear Hookean force law. Because the motion of the polymer would depend on its instantaneous configuration, Zimm linearized the problem and was able to make analytical progress by replacing G by its ensembled-averaged property at equilibrium. This process yields a model with the correct (HI-dominant) molecular weight scaling laws for diffusivity and polymer relaxation time but fails to describe polymer dynamics in nonequilibrium flow- conditions.

A refinement this "preaveraging approximation" involves averaging the HI tensors in the proper flow field. This so-called "consistent averaging model" is successful in predicting a shear thinning viscosity (η_p) and a nonvanishing (although positive at low shear rates) second normal stress coefficient (Ψ_2) in simple shear flow. However, this method ignores fluctuations in HI because it inherently involves an HI interaction tensor averaged over all configuations. Significant progress was made by Ottinger and independently by Wedgewood by assuming Gaussian distribution functions which leads to a closed set of equations for the ensemble-averaged second moment of the end-to-end vectors for bead—spring chains. This model gives good agreement with results from Brownian dynamics simulation for both η_p and Ψ_2 for Hookean dumbbells in shear flow. In addition to kinetic theory, Brownian dynamics simulation allows for solution of the equations of motion for the beads (without approximations) for large polymer chains with fluctuating HI.

It has for the most part been accepted that polymers with numerous constancy lengths might as well display noteworthy intramolecular hydrodynamic communications. In this respect, it is shocking that the free-emptying model exactly catches the dynamical stream conduct of lambda Dna as indicated in past studies. Later work27 demonstrated that consideration of hydrodynamic interactions and rejected volume (Ev) into a bead—spring polymer model gave not a qualitative or a calculable quantitive change in the transient or consistent atomic enlargement of lambda Dna in shear and planar extensional stream. Lambda Dna is a curious polymer in the accompanying sense: it is huge enough to display without non emptying conduct at harmony for instance, chain diffusivity scales as sub-atomic weight $M^{-0.6}$ in an exceptional dissolvable), yet sufficiently minor such that consideration of conformity ward drag is basically unnecessary for a quantitative portrayal of transient and relentless motion in shear or planar extensional stream. Hsieh et al. additionally achieve this conclusion observing lambda Dna utilizing Brownian elements reproductions with fluctuating Hi without barred volume interactions. Other exploratory confirmation additionally represents the bizarre dynamical conduct of lambda Dna. The fluctuating movement of part of the way augmented single lambda Dna atoms could be portrayed by eight straightly free typical modes. Nonetheless, the modal relaxation times display a Zimm-such as scaling, recommending that Hi impacts ought to be acknowledged at moderate polymer amplifications. For somewhat bigger Dna atoms give or take 4 lambda (126 ftm) long, reproductions of Jendrejack et al show that consideration of Hi marginally adjusts the transient sub-atomic reaction in planar extensional stream.

Recent experimental work by Schroeder et al. shows that extremely large chains of DNA ($L \approx 1.3$ mm, equivalent to $\approx 20\,000$ persistence lengths) were re quired to observe conformational hysteresis. On the basis of the results from this study, it is clear that HI can affect the nonlinear rheology of flexible polymers in a qualitatively different manner than previously expected. Conformation hysteresis and, more gener-ally, conformation-dependent drag may have a profound impact on the development of constitutive equations for polymer solutions and may be required for accurate modeling of turbulent drag reduction. Therefore, it behooves us to carefully study the effects of HI on polymer chain dynamics by taking advantage of non- equilibrium microstructural data from both single molecule experimental techniques and Brownian dynamics simulation.

- M. Doi. *J. Comp. App. Math.* 149. 13-25 (2002).
- OCTA. integrated simulation system for soft materials,
- T. Aoyagi, F. Sawa, T. Honda. M. Sasaki, Y. Nishio. *J. Soc. Rheology Jpn.* 30, 247-252 (2002).
- T. Aoyagi. F. Sawa, T. Shoji. H. Fukunaga, J. Takimoto. M. Doi. *Comput. Phys. Commun.* 145. 267-279 (2002).
- J. Takimoto, H. Tasaki, M. Doi. *Proceeding of XIIIth International Congress on Rheology*, p. 97 (2000).
- T. Honda. S. Urashita, H. Morita. R. Hasegawa, T. Kawakatsu, M. Doi. *Kobunshi Ronbunshu* 56, 762(1999).
- T. Yamaue, T. Taniguchi, M. Doi. In *Proceedings of AIP Conference, Statistical Physics*, M. Tokuyama and H. E. Stanley (Eds.), 519, 584 (2000).
- Aoyagi, T. Honda, M. Doi. J. *Chem. Phys.* 117. 8153-8161 (2002).
- Karl F. Freed. Functional integrals and polymer statistics. Advances in Chemical Physics, 22:1{128, 1972.
- Pierre-Gilles de Gennes. Scaling Concepts in Polymer Physics. Cornell University Press, 1979.
- Masao Doi and Sam F. Edwards. The Theory of Polymer Dynamics. Oxford University Press, 1986.
- Hiromi Yamakawa. Helical Wormlike Chains in Polymer Solutions. Springer-Verlag, 1997.
- Steven B. Smith, Yujia Cui, and Carlos Bustamante. Overstretching B{DNA: The elastic response of individual double{stranded and single{

stranded DNA molecules. Science, 271:795{799, 9 February 1996.

- Richard P. Feyman and Albert R. Hibbs. Quantum Mechanics and Integrals. McGraw-Hill, 1965.

- Khomami, K.K. Talwar, H.K. Ganpule, A comparative study of higher- and lower-order finite element techniques for computation of viscoelastic flows, J. Rheol. 38 (1994) 255–289.

- P.S.Doyle, E.S.G. Shaqfeh, G.H. Mckinley, S.H. Spiegelberg, Relaxation of dilute polymeric solutions following extensional flow, J. Non-Newtonian Fluid Mech. 76 (1998) 79–110.

- H.C. Öttinger, M. Laso, Smart polymers in finite element calculations, theoretical and applied rheology, in: P. Moldenaers, R. Keunings (Eds.), Proceedings of the International Congress on Rheology, Elsevier, Brussels, 1992.

- M. Laso, H.C. Öttinger, Calculation of viscoelastic flow using molecular models: the CONNFFESSIT approach, J. Non-Newtonian Fluid Mech. 47 (1993) 1–20.

- M.A. Hulsen, A.P.G. van Heel, B.H.A.A. van den Brule, Simulation of viscoelastic flows using Brownian configuration fields, J. Non-Newtonian Fluid Mech. 70 (1997) 79–101.

- P. Halin, G. Lielens, R. Keunings, V. Legat, The Lagrangian particle method for macroscopic and micro–macro viscoelastic flow computations, J. Non-Newtonian Fluid Mech. 77 (1998) 153–190.

- Ghosh, G.H. McKinley, R.A. Brown, R.C. Armstrong, An adaptive length scale method for dilute polymer solutions, in: Proceedings of the XIIIth International Congress on Rheology, Cambridge, UK, August 2000.