

# Research Proposal

In my research career, I have had a rich and varied range of projects to work on, and the proposal herein is likewise diverse with one common thread: For myself and those that join my group, I am interested in modeling the nonlinear dynamics of complex systems, with a special focus on rheological and biological systems. In regards to the former, I am interested in modeling industrially relevant deformation and flow of industrially relevant materials. In regards to the latter, I am interested in modeling population dynamics in ecosystems subjected to epidemics and/or invasive species. These two topics may seem like unusual companions but in both cases the underlying microscopic models are based on processes of birth/death, advection/diffusion, and relaxation/recovery - the supporting mathematics for the two fields are surprisingly similar in many respects. These topic are, in my view, a complementary pairing for a multidisciplinary research group studying non-linear dynamics of complex systems.

Most of my research career has been focused on constitutive modeling of complex fluids, especially entangled polymers. Complex fluids embody the ideal of low-cost and high value-added materials, and understanding the rheology of such systems (i.e. the response to processing and flow) is uniquely important for two reasons: (1) the value of a complex fluid is often derived from the microstructure that arises during the course of its processing [1, 2, 3], and (2) The very properties that make complex fluids valuable often make them challenging to process at high throughput [4, 5, 6], as needed for profitable production. Good constitutive models bridge the gap between knowledge of the microstructure and understanding of bulk flow behavior, and *vis* versa.

My foray into biological systems (and epidemic modeling in particular) began recently with work on COVID-19 [41], but my broader interest in the population dynamics of biological systems is much older. As the son of a forester, I grew up learning about the damage done by invasive species like zebra mussels [42], emerald ash borers [43], and purple loosestrife [44], as well as the potential risks and benefits of biological control strategies [45]. For native species, I also learned about problems of overpopulation in whitetailed deer [46] and population collapse in pollinators [13, 14]. In each of these examples - and many more around the world [15, 16, 17]- ecological models can help inform and improve the way that limited resources are deployed in ongoing efforts to preserve the health and vitality of our natural ecosystems.

With these motivations in mind, I outline three prospective research topics for consideration. First, there is an opportunity to fill a gap between theory and practice for high Reynolds number flows of many complex fluids. Second, I propose an example problem for modeling epizootic controls of invasive species. Third, I posit a new model system for studying the non-linear mechanics of dry entangled fibers and probing the fundamental physics of mechanical entanglement.

## 1. Reynolds Averaging for Complex Fluids

In recent decades, rheologists and soft matter physicists have made remarkable progress in building constitutive equations that connect the microscopic structure of a material to its bulk flow behavior. At one point, microscopically-derived constitutive models were only available for **very simple complex fluids**, such as dilute suspensions of hard spheres [18], droplets [19], and polymers [20]. Today, however, microscopically-derived constitutive models are available for all manner of complex fluids, including entangled linear polymers [21], wormlike micelles [22], dense suspensions [23], yield stress fluids [24], and even more exotic materials like entangled telechelic star polymers [25]. In principal, these models are useful for directly modeling **industrially relevant fluids under industrially relevant flow conditions**, but in practice this is not always true - many industrially relevant complex fluids (e.g. drilling muds, fracking fluids, emulsions, etc.) are processed at high Reynolds numbers.

At high Reynolds number, the chaotic “fluctuations” of a turbulent flow impart an additional level of “microstructure” to the fluid at length-scales and time-scales much smaller and much faster than those of the overall process. This, in turn, makes direct numerical simulation impractical - ideally, one would prefer to treat the turbulence itself as an additional level of microstructure to be averaged out.

The notion of turbulence as an additional level of microstructure (c.f. Figure 1) is used extensively for modeling Newtonian fluids at high Reynolds numbers [26, 27, 28], but at this point Reynolds-averaged constitutive models for complex fluids are mostly limited to simple approximations of simple fluids, like the FENE-P model for dilute polymer solutions [29]. The process of constructing Reynolds averaged constitutive equations is difficult in practice but straightforward in principal; just as particle-scale constitutive equations

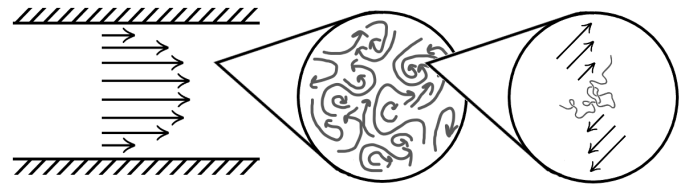


Figure 1: Turbulence as an additional layer of microstructure. Cartoon shows a polymer-based complex fluid as an example.

rely on closure approximations informed by particle-based simulations, Reynolds-averaged constitutive equations rely on closure approximations informed by direct numerical simulation of the particle-scale constitutive equation in simple turbulent flows.

As a starting point on this project, I would like to develop Reynolds-averaged constitutive equations for dense suspensions, leaning on recent work by Gillesse et. al. [23] to describe microstructure evolution at the particle-scale. I worked on this constitutive model during my post-doc, and I am convinced that it contains sufficient microscopic detail to be useful for turbulent flow modeling: the Gillesse models have been successfully validated in reversing flows [30] and flows with unsteady perturbations [23], for example. Immediate applications for a Reynolds-averaged extension could include modeling of drilling muds, industrial concrete mixers, mudslides, and more.

## 2. Ecological modeling (sample proposals)

The gypsy moth (Lepidoptera: Lymantriidae) is an invasive species that can cause enormous damage to ecosystems through defoliation of hardwood trees [31]. The moth was originally native to Europe, but was introduced to Massachusetts around 1870, whereafter it began to spread westwards [32]. In the early days, it was difficult to contain the spread of the gypsy moth population - there were few natural predators, and species-specific pathogens (e.g. *Lymantria dispar* multicapsid nuclear polyhedrosis virus or LdMNPV) are not a strong control method unless the moth population is already moderately high [33]. In this respect, viral controls were (and still are) helpful in the short term but not viable as a long-term control measure. Pathogens that are not species specific, like baculoviridae, can also be useful for short-term control of major outbreaks.

Today, the gypsy moth population continues to spread but it now poses a greatly reduced long-term risk to natural habitats, primarily due to a species-specific fungus from Japan (*Entomophaga maimaiga*) that was first established in New York in the late 1980s [34]. Unlike the viral pathogen LdMNPV, the fungal spores can persist in the environment for years, making it effective for long-term population control even when the moth population is low. At the leading edge of the gypsy moth invasion, however, this fungus is not yet established in the environment and there is still an abundance of foliage and an absence of natural predators. In the very long term, both the gypsy moth and its fungal pathogen will inevitably establish themselves across North America, and the fungal pathogen will keep population levels in check. But to reach this final state, what control measures best balance the total damage to our ecosystems against the total cost of containment? The question of optimal control is still an ongoing area of research.

To that end, I would like to use sophisticated new epidemic modeling tools (like those in the pyRoss library I worked on for COVID-19) to study optimal control measures in systems involving invasive species and two complementary control pathogens: one with a long persistence time but a low reproduction rate (e.g. the fungus) and another with a high reproduction rate but a low persistence time (e.g. the virus). The gypsy moth and its pathogens are an appealing system for a first application, but I believe that the general modeling framework may prove interesting for other invasive species, where long-term biological control measures are still a subject of active research (e.g. cane toads [17], emerald ash borers [43], and zebra mussels [42]).

A cartoon describing an idealized version of this problem with one spatial dimension is shown in Figure 2. At position  $x = 0$ , the moth and its fungus are both endemic, and neither poses a long-term threat to the native habitat. At position  $x = 1$ , neither the moth nor its fungus are present. The leading edge of the moth invasion occurs around  $x = 0.4$ , where the virus is being introduced (and reproduced by the moths themselves) to slow the invasion. This is, in a sense, a kind of multi-component reaction/diffusion problem, except the reactions (and potentially even the diffusion) are

biological processes with distinct kinetics and time-delays particular to the system of interest.

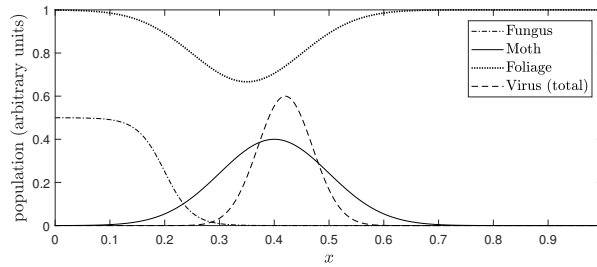


Figure 2: A cartoon figure for the spread of gypsy moths across a 1D landscape in the presence of fungal and viral control measures. Viruses are introduced (and reproduced) at the leading edge of the moth population to slow the spread, while a fungus trails the leading edge to keep the moth population in check long term. Defoliation (and the damage thereof) is primarily localized to the leading edge of the invasion.

### 3. Constitutive Modeling for Dry Entangled Fibers

What is a mechanical entanglement, and how do entangled structures change under non-linear deformation and flow? For constitutive modeling of well-entangled polymer melts, the depth and difficulty of these questions **have begun to make waves** that threaten confidence in the tube-based models upon which the whole field has been built [35, 36, 37]. The underlying discussion is fascinating and the implications are enormous, but I think it's possible that to answer the question as posed one must begin by considering an entirely different kind of system.

When dry fibers are matted together at sufficiently high concentrations, frictional interactions and non-crossing interactions between the fibers facilitate a rigidity percolation through a stretched mat of fibers. An entanglement is **unambiguously** identified by fiber/fiber contacts that participate in the rigidity percolation. By considering all possible deformation directions (and hence all possible rigidity percolations) one can unambiguously identify the full set of mechanical entanglements within the system. Under non-linear deformation, fibers will bend and slip, unambiguously releasing entanglements or activating incipient entanglements in the process. Thus, for non-linear deformations of dry fibers, one can define (and study) entanglements with a precision that may never be possible for well-entangled polymers.

It should also be noted that the non-linear mechanics of dry fibers is an interesting problem in its own right. The most popular constitutive equations (e.g. the Fiber bundle model) are quite old [38] but even modernized variations have only a passing connection to the microscopic structure of the fibers themselves [39, 40]. There is definitely room for improvement in the whole modeling framework, and the impact could span applications from textiles to re-inforced composites. Methods recently developed for underconstrained networks may provide an insightful framework for developing improved constitutive equations [41, 42, 43]. The principal difference is that, for entangled fibers, the connectivity network is

not defined by pre-existing linkages but rather created in the course of deformation.

As a first proposal, I would like to develop a constitutive model for densely matted C-shaped fibers (c.f. Figure 3). This is a highly artificial idealization of real fibers, but from a simulation and modeling standpoint it has clear advantages: it is the simplest possible system capable of forming entanglements without frictional interactions, and it is also trivial to describe how fibers change shape in response to an imposed stress. Fibers shaped like staples have been more extensively studied to-date [45, 46], but (for the reasons listed above) present a less promising framework for continued study, in my opinion. Once a mathematical framework is established for the model system of matted C-fibers, I would like to move towards systems with greater industry relevance - adding frictional interactions and polydispersity in fiber length/curvature.

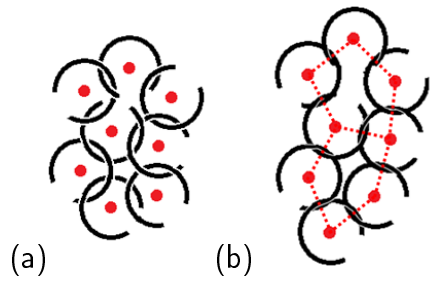


Figure 3: Cartoon of matted C-fibers before (a) and after (b) a non-linear deformation non-linear deformation

Overall, this project could have immediate impact on applications for processing/handling of dry fibers. Given the sphere of application over which existing fiber bundle models are currently in use, future applications of this work could extend to biological materials and fiber-reinforced composites [47, 48]. Perhaps somewhat optimistically, I also believe that this work could bring much-needed clarity to broader questions about the physics of mechanical entanglement in a broader class of materials (e.g. fiber suspensions, polymer melts, etc.).

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