erogeneity Quantification in dynamical systems consisting of (many) individual dynamical units coupled in a network. These units di er in the way they are structurally linked to form the network; their “structural identities” are heterogeneous, and the distribution of these heterogeneities derives from the network structure itself.

Network models are increasingly being used to study large, complex real life systems in a variety of contexts such as the internet, chemical and biochemical reaction networks, social networks and more [2, 3, 4, 5, 6]. A network is a mathematical representation of individual subsystems called nodes (or vertices), which are connected to one another through edges (or links). In the specific example of a social network the nodes represent people, while the edges connecting them represent relationships (friendships, coauthorships, etc.) between them. The following references provide useful reviews of basic network concepts and of the study of dynamics of evolving networks [7, 8, 9, 10, 11, 12].

a known distribution on uncertain dynamical systems [19], and we will discuss this analogy in more detail below.

In order to illustrate these ideas we consider a simple agent-based model of opinion propagation where the agents are connected by a social network; simulations of this model indicate that the states of the agents become quickly correlated to the connectivity degrees of these agents as nodes in the network. The paper is organized as follows: Our illustrative model is described in Sec. 2, along with a quick overview of its nonlinear dynamic behavior. Sec. 3 defines and describes the coarse representation that forms the basis of our computational reduced model. A few details of the coarse variable description are relegated to the Appendix, in order to maintain the simplicity and flow of the discussion. A brief outline of the Equation-Free approach employed to computationally implement the reduced model is described in Sec. 4, along with the results of

Figure 1: Left: The degree histogram of the illustrative network structure

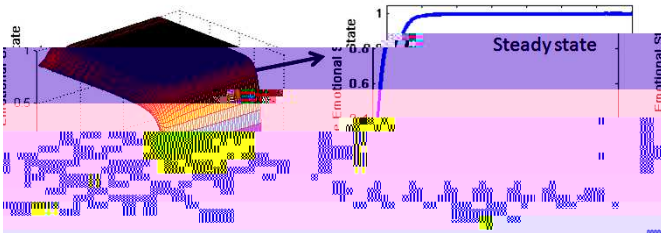

Figure 2: A $3D$ plot of the evolution of the average emotional state of agents with a given degree versus the degree is shown evolving over time on the left. The steady state of this average emotional state versus degree is shown on the right. The initial condition for the simulation gave all agents a uniform emotional state of 0.8.

2.1. Nonlinear model behavior

The dynamical behavior of the model is described in considerable detail in [20]. We briefly recount some basic features of these dynamics here. Direct simulations, using the model rules, initialized at different initial conditions are presented. The state of the system at any moment in time is completely specified by the states of each of the $20,000$ agents in the network. Certain properties of the system can be best conveyed through chosen collective observables that are hopefully representative of the overall dynamics of the system. The average emotional state of all network agents is one such observable of interest. The evolution of average emotional state of all the agents in the network from various distinct initializations is shown in Fig. 1; for simplicity, the states of all the agents were initialized uniformly at fixed values over the network (but different fixed values for each initialization). The figure shows that the system reaches one of three stable steady states depending on the initial conditions; parameter settings leading to a single stable, or to two stable stationary states also exist in a detailed bifurcation diagram and have been discussed in [20].

3. Coarse representation

To obtain a reduced model, one must first select a set of coarse variables that accurately capture the long-term evolution of the system. To motivate our choice, we examined the detailed profiles of system states along an ensemble of trajectories like the ones summarized in Fig. 1. For this model, we observed that the states of the agents quickly become highly correlated with their degrees. Fig. 2 shows the evolution in time of the average state of all agents in a degree class (i.e., all agents having the same degree) as a function of the degree. The curve evolves smoothly in time, and it was demonstrated in [20] that such a correlation could indeed be used to obtain a reduced description of the model. A method of "binning" was employed in that work to construct good collective variables: this involved partitioning the network nodes into different groups (based on the node degrees) and required 80 such groups, leading to 80 coarse variables.

We now realize that what, in that paper, was an ad hoc reduction is just a special case of a very general, and potentially powerful approach to systemati-

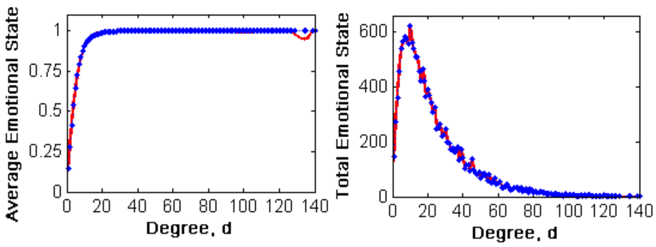

Figure 3: Left: **The steady state average emotional state of all the agents with a specified degree (as in the right plot of Fig. 2) is plotted versus the degree as (blue) dots. The curve fit obtained by using 10 of our orthogonal polynomials is plotted as a (red) solid curve for comparison.** Right: **For the same case, the total emotional state of all the agents with a specified degree is plotted versus the degree as (blue) dots. This plot on the right is just a product of the plot on the left and the degree histogram shown in Fig. 1. The (red) solid lines correspond to the results from our polynomial approximation procedure.**

in the approximation procedure. We choose simple proportional weights which implies $w(d) = h(d)$, where $h(d)$ represents the histogram of degrees (i.e., $h(d)$ is the number of agents in the network with degree d).

The polynomials p_i are thus chosen to be orthogonal with respect to the degree distribution $h(d) = w(d)$. This orthogonality condition can be described as follows:

$$\langle p_i(d), p_j(d)\rangle_{w(d)} = \delta_{ij}. \quad (3)$$

Since the polynomials are orthogonal with respect to the weight distribution, the coefficients that minimize the residual (with respect to the same weights) in Eq. 2 can be directly evaluated by the following simple expression:

$$c_i = \langle p_i(d), f(d)\rangle_{w(d)}. \quad (4)$$

scheme suggests Meixner polynomials as basis functions. The derivation of orthogonal polynomials for any (discrete, possibly truncated/empirical) weight function w(d) (which we used for our numerical computations) is discussed in the Appendix.

In Fig. 3, we re-plot the curve of average emotional state versus degree at the "top" steady state branch (steady state 1 in Fig. 1) using (blue) dots. We evaluate the first 10 polynomials that are orthogonal to the degree distribution of our particular network, sampled empirically from the "theoretical" truncated geometric distribution. The corresponding a1.66638(t)2.56084(io)-5.8887(n)0.9313121.66(a1.2v)21.1263(e operator can then be defined in terms of this microscopic evolution operator as well as the lifting and restriction operators as follows:

$$\Phi_t(\cdot) = R \circ \varphi_t \circ L(\cdot). \tag{5}$$

In other words, the evolution of the coarse variables can be represented as:

$$\mathbf{c}(T + t) = \Phi_t(\mathbf{c}(T)),$$

where Φ_t is defined in Eq. 5 and $\mathbf{c}$ represents the vector of coefficients $[c_1, c_2, \ldots c_k]$.

W0236lIu929988(s)-3.4847(,)-.56084(r)-6.48664(a)-5.89115(t)2.56329(e)-1.6,e ve.0.928763(d)p326.863(v

Figure 4: Evolution of the coarse variables corresponding to Fig. 2. The solid lines indicate results obtained from direct simulations. The dots indicate results obtained through coarse projective integration using 10 coeﬃcients (accelerating the overall simulation by a factor of 2) The plot on the left shows the evolution of the first 5 coeﬃcients, while the plot on the right shows that of the next 5 coeﬃcients.

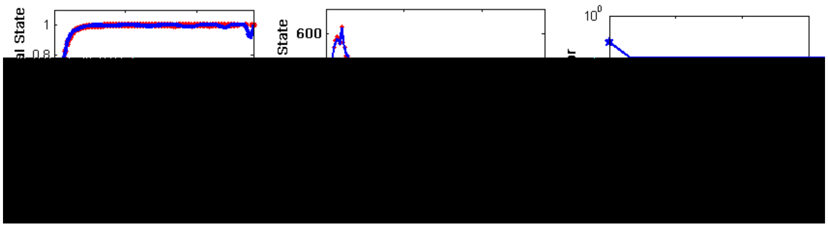

Figure 5: Left: The steady state average emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by New[illegible]

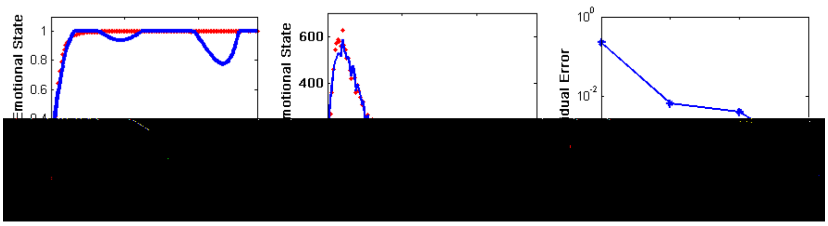

Figure 6: Left: **The steady state average emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve.** Center: **The steady state total emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve.** Right: **Convergence of Newton-GMRES: The L_2 norm of the coarse residual is plotted against the iteration number. Computations were performed with a 6 polynomial**

“Heterogeneity Quantification” rather than Uncertainty Quantification. In UQ problems, the effect of a random parameter with a known distribution on the system state is captured by expanding the state in terms of orthogonal polynomials of the random variables. The orthogonal polynomials used depend on the distribution from which the random variables are sampled. In our case, the states of the agents depend on the agent structural identities (here, agent degrees, whose distribution is prescribed by the network) -and, of course, on time. By analogy, we can think of the degrees as a “random heterogeneity parameter” with a given distribution, and parsimoniously capture its effect on the agent states by expanding the states in terms of suitable orthogonal functions of the degree. It is clear that the approach can be extended to states that depend on “higher order” structural identities - identities that do not only depend on the degree, but also on more/different network statistics: for example, degree and clustering coefficients for each node. The joint distribution of these latter two features will again be dictated by the network, and the basis functions will be now two-dimensional - clearly, the integrals involved in computing the corresponding coefficients will start becoming cumbersome as the number of “determining features” grows. For such problems, there has already been considerable progress on collocation-based computations, and the use of sparse grids in the UQ literature [27, 28, 29] and we expect that these tools will also become useful in network coarse-graining when multiple network features affect the system state. Still, there is no reason for the roots of polynomials orthogonal with a given degree distribution weight to be themselves integers, and so collocation approaches to approximating integrals over degree distributions must be addressed.

connected with a node of degree k_j; they also considered the case of no assortativity. In our case, we do not derive such equations explicitly, but we solve them through our equation-free approach. All our computations above were performed with a fixed, static network, with a particular, prescribed degree distribution; choosing that particular network, also de facto selected all additional high order statistics through the network construction (including a particular assortativity). In that sense, our equations constitute a coarse-graining of the particular network.

It is also conceivable that one may want to construct (and average over) several sample networks a research visit to Princeton.

Appendix A. Finding a suitable basis of orthogonal polynomials tailored to a given degree distribution

The procedure that we use to evaluate a set of polynomials orthogonal to one another with respect to an empirical weight distribution [33] (defined over a range of integers, here the node degrees) is described here. Let the i-th required polynomial be denoted by p_i, and let $w(d)$ be the specified discrete weight distribution. p_i can be written using the following general representation:

$$p_i = \alpha_i \left(1 + \sum_{j=1}^{i-1} y_{ij} d\right). \tag{A.1}$$

The orthogonality condition is written as

$$\langle p_i, p_j \rangle_{w(d)} = \delta_{ij}. \tag{A.2}$$

Since we are interested in evaluating the function at discrete values of d, we may approximate the orthogonality condition by the following summation:

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