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An Individual-Based Approach for Studying System-Wide Properties of Ecological Networks

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13.1 Introduction

Ecological networks are widely used to represent the biotic interactions in an ecosystem, such as the movement of biomass in consumer-resource systems, transfer of energy in food webs, and carbon cycling in the biosphere. Ecological network models are built to describe the flow of biomass or energy within ecosystems. Network Environ Analysis (NEA) (Patten, 1978; Fath and Patten, 1999) formulates system-wide properties to describe various relations in an ecosystem. For example, cycling index quantifies how much of the energy or biomass is recycled and throughflow analysis measures how the environmental inputs contribute to the throughflow of each compartment. Computation of most of these properties relies on formulations based on linear algebra. These algebraic formulations are only applicable to ecosystems at steady state, which are rarely seen in the environment. Dynamic ecosystems are more common as ecosystems are often driven by seasonal changes and as unexpected regime shifts or environmental impacts can occur. The purpose of this work is to extend the applicability of these useful but limited properties to dynamic ecosystem models.

Network Particle Tracking (NPT) is an individual-based method that simulates system dynamics. It works like an *in silico* version of tracer experiments by simulating pathways of traced elements. As an alternative to algebraic formulations of NEA properties, we construct simulation-based formulations that compute the same NEA properties. While these new parallel definitions for NEA properties agree with conventional methodologies on steady-state systems, they are also applicable to dynamic models.

In this chapter, we first provide a brief introduction for NEA, followed by a description of how NPT simulates ecosystem models. We then focus on formulating NPT-based

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definitions for various ecosystem properties such as cycling index, throughflow analysis, and storage analysis. Finally, we discuss how NPT-based definitions can be used to compute dynamic network properties, and demonstrate this methodology on storage analysis.

13.2 Network Environ Analysis

Leontief (1951, 1966) developed the input–output analysis to analyze the interdependence of different branches of national economy. This analysis was introduced to ecology by Hannon (1973). NEA (Fath and Patten, 1999; Patten, 1978) uses the same idea of economic input–output analysis to study environmental systems. Ecosystem models are represented as individual compartments connected by pairwise links. NEA methodology formulates various measures that describe the relationship between these compartments and the environment. NEA consists of two main analyses: (i) structural analysis and (ii) functional analysis. The former investigates the direct and indirect connections from one compartment to another, and is also the basis for the functional analysis. The functional analysis quantifies the relationship between the compartments and the environment and includes throughflow, storage, and utility analyses.

NEA works with compartmental models representing ecosystems. Figure 13.1 shows a hypothetical system with three compartments. Each circle represents one compartment, which corresponds to a part of the system. The arrows represent environmental inputs/outputs or flows between compartments. Depending on what ecological process is modeled, the flow currency could be biomass, energy, or a specific nutrient or element.

NEA stores both the qualitative and quantitative information of the network in matrices and vectors. For the simple model in Fig. 13.1, the environmental inputs (z), outputs (y), and storage values (x) are defined as follows:

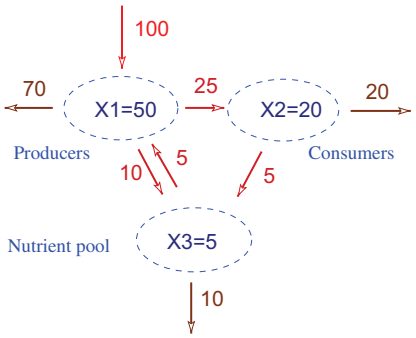

FIGURE 13.1 A hypothetical three-compartment ecosystem model consisting of *Producers*, *Consumers,* and *Nutrient pool* with stocks X1 = 50, X2 = 20 and X3 = 5 units, respectively. These three compartments are connected

$$z = \begin{bmatrix} 100 \\ 0 \\ 0 \end{bmatrix} \quad y = \begin{bmatrix} 70 \\ 20 \\ 10 \end{bmatrix} \quad x = \begin{bmatrix} 50 \\ 20 \\ 5 \end{bmatrix}$$

z_i : Rate of enviornmental input to compartment i

y_i : Rate of environmental output leaving compartment i

x_i : Storage value of compartment i

Adjacency matrix A consists of zeros and ones. A_{ij} indicates if there exists a direct flow from compartment j to compartment i. A matrix represents all connections within the system. In addition to the connectivity information, **flow matrix** F describes how strong the connections are. F_{ij} denotes the rate of direct flow from j to i. A and F matrices for the simple ecosystem model in Fig. 13.1 are:

$$A = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix} \quad F = \begin{bmatrix} 0 & 0 & 5 \\ 25 & 0 & 0 \\ 10 & 5 & 0 \end{bmatrix}$$

Throughflow T_i is the rate of material (or energy) moving through compartment i. It is defined as the sum of flows to compartment i from other compartments and the environment (T_i^{in}). For a system at steady state, it equals the sum of flows from compartment i to other compartments and the environment (T_i^{out}):

$$T_i^{\text{in}} = \sum_{j=1}^{n} F_{ij} + z_i \quad T_i^{\text{out}} = \sum_{j=1}^{n} F_{ji} + y_i$$

For this simple model,

$$\mathbf{T}^{\text{in}} = \mathbf{T}^{\text{out}} = \begin{bmatrix} 105 \\ 25 \\ 15 \end{bmatrix}$$

Finally, **total system throughflow** (TST) is defined as the sum of all compartmental throughflows in the system:

$$TST = \sum_{i=1}^{n} T_i = 105 + 25 + 15 = 145$$

Current NEA methodology and various properties involved are developed for steady-state systems. All the matrices and vectors involved in the computation of these properties are required to be constants, not functions of time. Little work exists on NEA applied to evolving systems (Hippe, 1983; Shevtsov et al., 2009). Hippe (1983) states "it would be desirable to develop a nonlinear environ analysis for either general or specific classes of nonlinear systems. Although such an analysis would not be isomorphic to the analysis presented herein, certainly there would exist analogous formulations of concepts between these two types of analysis." Shevtsov et al. (2009) describes a methodology applicable to dynamic systems; however, there are limitations in its accuracy and

convergence. The methodology presented in our work is general, and is valid for models with linear or nonlinear flows, and time-invariant or time-dependent coefficients.

13.3 Network Particle Tracking: An Individual-Based Methodology

NPT is an individual-based simulation method. Energy (or mass) entering the system is divided into small packets, and each packet is labeled and tracked in time as it flows through the network. Figure 13.2 uses a simple three-compartment model to illustrate the working of NPT. It starts with breaking initial stocks or input flows into discrete packets, which we call "particles". For example, for a carbon flow model, a particle could represent a single C atom, or 1 gram of Carbon. This choice is left to the modeler. The smaller the particle, the more the computational resources required for the simulation. In principal, it is preferred to use the smallest possible unit allowed by computational resources. Based on flow rates, NPT determines which flow is likely to occur and when. A particle is then chosen randomly from the donor compartment and introduced to the recipient compartment. As ecosystems are open systems, new particles will enter the system. So if the chosen flow is an environmental input, a new particle is labeled and introduced to the recipient compartment. NPT simulation output includes the history of the movements of all particles within the system.

Figure 13.3 shows a partial NPT simulation output for the three-compartment system (from Fig. 13.2), which includes the pathway, flow time, and residence time data. The

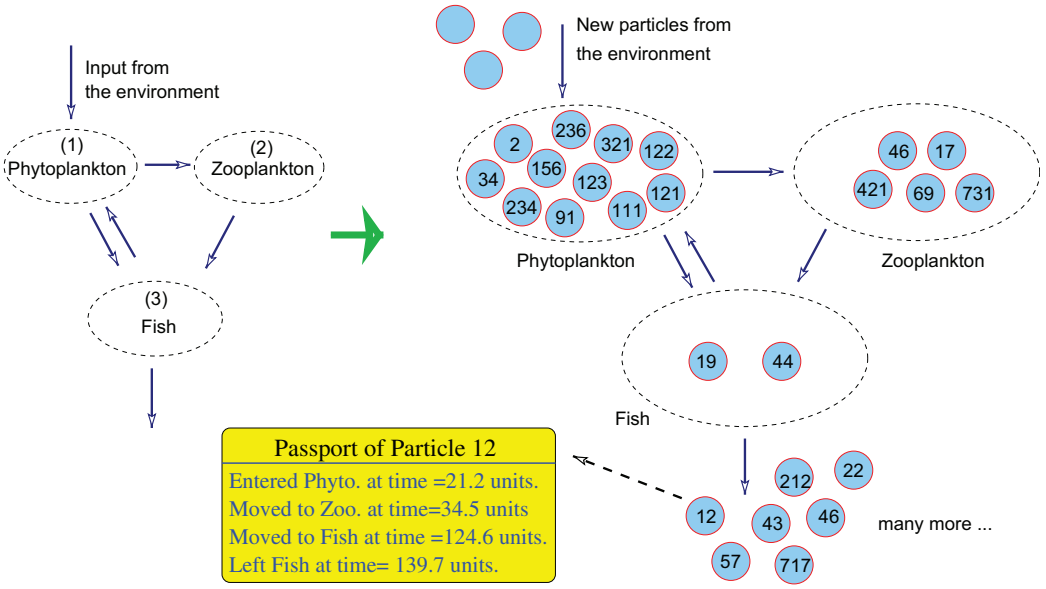

FIGURE 13.2 Three-compartment model depicting particles and their flow information in the system. For color version of this figure, the reader is referred to the online version of this book.

pathway of a particle is defined as an ordered list of compartments visited by that particle. Flow time data shows when each particle flows from one compartment (or the environment) to another compartment (or the environment). Residence time data records how long a particle stays in a compartment it visits. For example, Fig. 13.3 represents the fact that "Particle 12" entered *Phytoplankton* (compartment 1) at time = 21.2, left at time = 34.5, and spent 13.3 time units in *Phytoplankton*. The time unit is determined by the modeler.

NPT is a discrete and stochastic method with several advantages over ordinary differential equation (ODE) models. However, ecological networks are often modeled using ODEs, which are deterministic and continuous. The same initial conditions for an ODE model will always generate exactly the same outcome, which is usually not the case in real life. On the other hand, stochastic models represent the inherent fluctuations in real-life systems by adding noise derived from a probability distribution, and therefore outcomes are not unique.

Another issue with the ODE models is that all flows are treated as continuous processes, which is not always appropriate. Take the simple food chain as an example.

$$\text{Tree} \rightarrow \text{Deer} \rightarrow \text{Wolf}$$

Assuming the deer could obtain leaves almost anytime, the flow from *Tree* to *Deer* can be approximated by a continuous process. However, it is not appropriate to regard the flow from *Deer* to *Wolf* as continuous since wolves attack deers occasionally. Once they succeed, a large amount of energy is moved from *Deer* to *Wolf* in a short period of time. It is preferable to model such rare and instantaneous processes with discrete, rather than continuous models.

NPT is based on the Gillespie algorithm (Gillespie, 1977), which is an exact stochastic simulation method. As described earlier, it discretizes material flows as movements of particles among compartments. For the simple food chain above, it is possible to represent the flow from *Tree* to *Deer* and *Deer* to *Wolf* with small and large-sized particles, respectively. In other words, the flow from *Tree* to *Deer* could be modeled using small-size particles (e.g., 1 gram of Carbon), while the flow unit from *Deer* to *Wolf* could be modeled

Particle 12	Pathway	* → 1 → 2 → 3 → *
	Flow time	21.2 34.5 124.6 139.7
	Residence time	13.3 90.1 15.1
Particle 43	Pathway	* → 1 → 3 → 1 → 2 → 3 → *
	Flow time	30.4 50.3 65.8 88.4 115.3 140.2
	Residence time	19.9 15.5 22.6 26.9 24.9
Particle 212	Pathway	* → 1 → 2 → 3 → 1 → 3 → *
	Flow time	31.2 50.3 79.8 98.0 123.5 131.6
	Residence time	19.1 29.5 18.2 25.5 8.1

FIGURE 13.3 Partial NPT output for three-compartment ecosystem in Fig. 13.2, including pathway, flow time, and residence time data. The numbers of 1, 2, and 3 correspond to compartments *Phytoplankton*, *Zooplankton*, and *Fish*. For color version of this figure, the reader is referred to the online version of this book.

as numerous small particles bound together, to represent the entire deer. This modified model represents the food chain better than just moving all particles independently.

NPT is a stochastic method compatible with the master equation (Gillespie, 1992, 2000). In other words, the mean of many NPT results agrees with differential equation solution. Therefore, studies based on NPT simulations, which are stochastic and discrete, are compatible with the conventional methodologies, which are often continuous and deterministic.

13.4 Cycling Index

Cycling index is an essential ecological indicator used for ecosystem analysis. It measures how much of the environmental input is cycled before exiting the system. Finn's cycling index (Finn, 1978) is widely accepted as an accurate measure of cycling within an ecosystem. The definition of Finn's cycling index relies on throughflow analysis. Therefore, here, we briefly introduce the throughflow generating matrix N, but postpone a more detailed description to the next section. N_{ij} represents the throughflow generated at i by per-unit input at j.

By definition, diagonal values of throughflow generating matrix N_{ii} represent the amount of throughflow generated at compartment i by one unit input into compartment i. This one unit input into compartment i contributes to its throughflow (T_i) at least once. Therefore, if N_{ii} is larger than 1, then $N_{ii} - 1$ represents the amount of throughflow generated at compartment i through cycling. Finn (1977, 1978) defines his cycling index based on this idea as the fraction of the total system throughflow (TST) that is due to cycling ($\mathrm{TST_c}$). For an ecosystem model at a steady state, **Finn's cycling index** (FCI) is defined as follows:

$$\mathrm{FCI} = \frac{\mathrm{TST_c}}{\mathrm{TST}} = \sum_{i=1}^{n} \left(\frac{T_i}{\mathrm{TST}} \frac{N_{ii} - 1}{N_{ii}} \right) \tag{1}$$

Here, n is the total number of compartments in the ecosystem model. By definition, the range of $\mathrm{TST_c}$ values are between zero and TST, therefore FCI varies between zero and one. This definition of FCI is applicable only to systems at steady state, where T, N, and TST are constants. We define an alternative, simulation-based definition for FCI, which is applicable to dynamic ecosystems as well. This definition is more intuitive, and does not require throughflow analysis or linear algebra.

NPT simulations generate the pathway data of individual particles within the system. Each compartment visit of a particle contributes to TST. Therefore, using the pathway data, TST represents the total number of visits to compartments by particles. And $\mathrm{TST_c}$ is computed as the number of compartments visited by a particle more than once. Therefore, we can quantify cycling in an intuitive manner using particle pathways. Table 13.1 demonstrates the computation of FCI based on the partial pathway data provided in Fig. 13.3.

In Table 13.1, the second column lists the compartments visited by each particle, and we underline compartments visited by a particle more than once. TST values are computed by counting the number of compartments visited by each particle. TST_c values are computed by counting the number of underlined compartments, which represent throughflows due to cycling. Therefore, the simulation-based cycling index is computed as: $FCI = \frac{TST_c}{TST} \approx \frac{4}{13} = 0.31$.

The result of this computation is based on the specific pathway data used, and therefore different pathway data sets will produce different results. In general, the larger the pathway data set, the higher the accuracy of the computed cycling index. Since NPT is based on a stochastic algorithm, the pathway data generated for each simulation will be different. However, as the pathway data size increases, the simulation-based FCI converges to its conventional definition in Eqn (1).

Kazanci et al. (2009) demonstrates the accuracy and convergence of the NPT-based FCI using the Hubbard Brook temperate forest ecosystem model (Finn, 1980). The flow currency in this model is Calcium, which explains the relatively high cycling index of 0.797. Figure 13.4 shows NPT-based FCI values computed for three different simulations.

Table 13.1 Computing of an Approximate Cycling Index for the Three-Compartment Model, Using Partial Pathway Data in Fig. 13.3

Particle	Pathway	TST	TST_c
12	1 2 3	3	0
43	1 3 1 2 3	5	2
212	1 2 3 1 3	5	2
Total		13	4

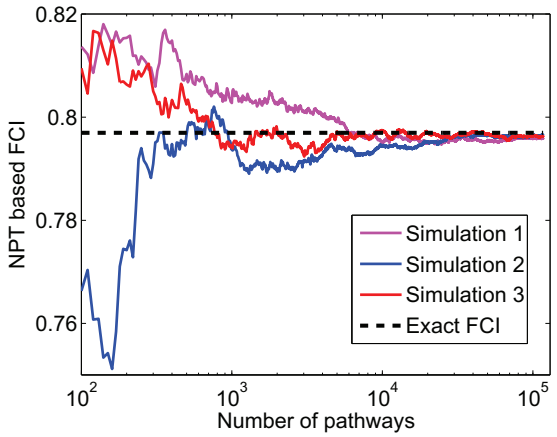

FIGURE 13.4 Finn cycling index is computed using the pathway data generated by three different NPT simulations for Hubbard Brook temperate forest ecosystem. For color version of this figure, the reader is referred to the online version of this book.

We observe that as pathway data size increases, the NPT-based FCI converges to the value computed with the conventional methodology, shown with the horizontal dotted line. The agreement of the two definitions reveals the meaning of FCI on an individual-based context.

13.5 Throughflow Analysis

Throughflow analysis investigates the relationship between environmental inputs and compartmental throughflows. Throughflow analysis consists of the **throughflowgenerating matrix** N, which is a linear mapping from the input vector z to the throughflow vector T, as shown in $Nz = T$. Throughflow analysis is an essential part of NEA, and is the basis for other system-wide properties such as cycling index (Finn, 1977, 1978, 1982) and indirect effects ratio (Higashi and Patten, 1986; Patten, 1986, 1985).

N_{ij} represents the throughflow generated at compartment i by one unit environmental input at compartment j. Using NPT, we could regard this unit input as one particle, and simulate its movement within the system. The definition then becomes the number of times a particle goes through compartment i given that it enters the system at j. Since NPT simulations provide pathways of particles as shown in Fig. 13.3, such computation becomes feasible. To compute N_{ij}, we use all pathways starting at j, which correspond to those particles entering the system at j. Then, we count the occurrences of compartment i in these pathways. The average number of occurrences of i for all particles defines the NPT-based N_{ij}.

However, for many ecosystem models, not every compartment receives environmental input. This is a problem because N_{ij} cannot be computed unless compartment j receives environmental input. To compute the full N matrix, we use the fact that whether a particle enters a compartment from the environment or from another compartment, it does not matter and it will behave the same way afterwards. In other words, we need not make any distinction between environmental inputs and inter-compartmental inputs to compute N. Therefore, we can treat each particle pathway as a set of multiple particle pathways as shown in Fig. 13.5. We name this new set **contracted pathways**.

This increase in the number of effective pathways also increases the accuracy of computation of N. The application of this expansion to all three pathways in Fig. 13.3 results in 10 new pathways, yielding 13 pathways in total. Using these 13 contracted pathways, we compute N_{31} in Table 13.2. Five of these 13 contracted pathways start with compartment 1. Compartment 3 appears seven times in these five contracted pathways, then N_{31} is computed as $\frac{7}{5} = 1.4$.

This method can be generalized to compute the entire N matrix based on a larger pathway data set that belongs to any compartmental ecosystem model, as follows:

$$N_{ij} = \frac{1}{|P_j|} \sum_{p \in P_j} \text{number of occurances of compartment } i \text{ in } p \tag{2}$$

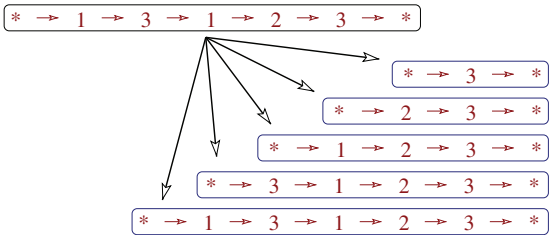

FIGURE 13.5 Pathway of particle 43 from Figure 13.3 is expanded into five separate contracted pathways. Such expansion enables us to compute N_{ij} and S_{ij} (in next section) even if there is no environmental input into some compartments. For color version of this figure, the reader is referred to the online version of this book.

Table 13.2 Computation of N_{31} Using the Partial NPT Simulation Output from Fig. 13.3

Particle	Pathways	Contracted Pathways Starting with 1	Number of Occurrences of 3
12	1 2 3	1 2 3	1
43	1 3 1 2 3	1 3 1 2 3	2
		1 2 3	1
212	1 2 3 1 3	1 2 3 1 3	2
		1 3	1
Total		5	7

where P_j is a list of contracted pathways that starts with compartment j, and $|P_j|$ represents the number of contracted pathways on this list. The larger the value $|P_j|$, the more accurate the computation of NPT-based throughflow generating matrix N.

Similar to NPT-based FCI, the NPT-based N matrix will converge to its conventional definition as more pathway data is used in its computation. Matamba et al. (2009) includes similar convergence and accuracy information for NPT-based N as we show for cycling index in Fig. 13.4. However, the method presented in this chapter is based on contracted pathways, and is an improved version of the methodology presented in Matamba et al. (2009). This new method converges much faster using less pathway data, increasing accuracy. Similar to FCI, conventional throughflow analysis is only applicable to steady-state ecosystem models. The NPT-based methodology can compute N matrix for pathway data that belong to dynamic systems, eliminating this limitation. Furthermore, this alternative definition of the N matrix is more intuitive, and confirms the conventional algebraic formulation of N.

13.6 Storage Analysis

Storage analysis (Matis and Patten, 1981) investigates the relation between input flows and compartment storage values. The **storage generating matrix** S represents a linear

mapping between the environmental input rates (z) and the storage values (x) of each compartment at the steady state, which is described by the equation $Sz = x$. For instance, given one unit of mass or energy input to a system at compartment j, S_{ij} represents how much storage is generated at compartment i as a result.

Storage analysis is conceptually the same as the throughflow analysis. Both measures map the input to compartmental values. To compute throughflow generating matrix N, we count the number of times a particle goes through a compartment using the pathway data. In storage analysis, the number of visits is replaced by the particle's total residence time in that compartment. The longer a particle resides in a compartment, the larger its contribution to the storage of that compartment. NPT simulations provide not only the list of compartments a particle visits, but also the duration of each visit. This additional information enables the computation of the S matrix in a similar way to that of the N matrix.

To compute S_{ij}, we use all pathways starting at j, which correspond to those particles entering the system at j. Then, we sum up their residence times at i. We compute S_{ij} as the average residence time at i for all particles.

Similar to throughflow analysis, the process of computing the S matrix is slightly more involved because an ecosystem model will rarely have environmental inputs into all its compartments. For example, we cannot compute S_{32} if no particle enters compartment 2 from the environment. To solve this problem, we carry out the computation of S on contracted pathways like what we did for computing N matrix. Since all compartments receive an environmental input and/or at least one inter-compartmental input, it is possible to compute the full S matrix for any ecosystem model.

To demonstrate the NPT-based definition of S, we compute S_{31} using the pathway data provided in Fig. 13.3. First, we determine how many contracted pathways start with compartment 1. Table 13.2 shows that five contracted pathways start with compartment 1. Using the residence time information in Fig. 13.3, we compute the total residence time at compartment 3 for these five contracted pathways. For example, the first contracted pathway ($\rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow *$) goes through compartment 3 once, and its residence time at compartment 3 is 15.1 time units. The second contracted pathway ($\rightarrow 1 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow *$) visits compartment 3 twice, staying for 15.5 and 24.9 time units, respectively. So, its residence time is the sum of these two values. Then, S_{31} is computed as follows:

$$S_{31} = \frac{(15.1) + (15.5 + 24.9) + (24.9) + (18.2 + 8.1) + (8.1)}{5} = 22.96$$

In general, we compute S as follows:

$$S_{ij} = \frac{1}{|P_j|} \sum_{p \in P_j} \text{sum of residence times at compartment } i \text{ in } p \tag{3}$$

where P_j is a list of contracted pathways that start with compartment j. $|P_j|$ represents the number of contracted pathways on this list. The larger the value of $|P_j|$, the more accurate the computation of NPT-based S. Convergence of the NPT-based S matrix to the conventional S matrix is discussed in Kazanci and Ma (2012), and the results are similar to that of the throughflow analysis and FCI.

13.7 Dynamic Network Environ Analysis

In previous sections, we demonstrated the NPT-based methodology to study several network properties. NPT-based definitions of network properties depend solely on the output of an NPT simulation, which consists of particle pathways and residence times. This simulation may belong to an ecosystem at a steady state, in transition to a steady state, oscillating between states, or even a chaotic system. Therefore, NPT-based definitions can be computed for dynamic ecosystems, unlike the conventional definitions of these measures, which are only limited to steady-state systems.

The NPT-based definitions introduced previously only allow us to compute constant values that represent the "average" behavior of a dynamic system over a time interval. In this section, we describe how to extend NPT-based definitions to compute time-varying network properties. We demonstrate this new technique on storage analysis. However, the process described here to extend the applicability of storage analysis to dynamic systems can be adapted to any NPT-based ecosystem property, including throughflow analysis and cycling index.

Our aim is to compute a true dynamic storage analysis matrix function $S(t)$, where $S(a)$ represents the instantaneous storage generating matrix at time $t = a$. To construct an NPT-based formulation for $S(t)$, a rigorous definition for $S_{ij}(t)$ is needed. Let $S_{ij}([a, b])$ represent the amount of storage created at compartment i over time ($[a, \infty]$), by per-unit input into compartment j over the time interval $[a, b]$. Then, we define the dynamic storage-generating matrix function $S(t)$ as follows:

$$S(t) = \lim_{h \to 0} S([t-h,\ t+h]) \tag{4}$$

In this definition, the storage contribution can occur at anytime. However, since environmental models are open and dissipative systems, all particles leave the system sooner or later. Therefore, we can revise the definition of the above $S_{ij}([a, b])$ and use an arbitrary large number M instead of ∞ ($[a, M]$instead of $[a, \infty]$).

Utilizing this new definition for dynamic storage analysis, it is now possible to compute $S(t)$ based on the output of NPT simulations. Similar to numerical differential equation solutions (e.g., Euler, Runge-Kutta, etc.), the NPT-based computation of $S(t)$ will employ a discrete time-step value h. Smaller h values are preferred for higher accuracy. To compute an approximate value of $S_{ij}(t)$, we first set a time interval $[t-h,\ t+h]$. Then, we label those particles that enter compartment j during this time period, and sum up their storage contribution to i. A detailed description of this process is as follows:

Step 1: Simulate the model with NPT until all the particles that move during the time window $[t-h,\ t+h]$ leave the system.

Step 2: To compute $S_{ij}(t)$, we find out all contracted pathways of the form

$$\rightarrow j \rightarrow \cdots \rightarrow i \rightarrow \cdots \rightarrow *$$

where the first flow "$\rightarrow j$" occurs during $[t-h,\ t+h]$.

Step 3: To get an estimated value for $S_{ij}(t)$, we add up all residence times at i for each contracted pathway, and divide this sum by the number of contracted pathways. This value is the storage contribution (at i) of a unit environmental input at j.

To demonstrate this process, we compute S_{31} over the time interval $[30,\ 32]$ using the sample NPT output provided in Fig. 13.3. The result will be an approximate value for S_{31} at $t = 31$. As described in Step 2, we focus on the contracted pathways of the form $\rightarrow 1 \rightarrow \cdots \rightarrow 3 \rightarrow \cdots \rightarrow *$. Based on the three pathways shown in Fig. 13.3, we totally get 13 contracted pathways (three for particle 12, five for particle 43, and five for particle 212). Five of these contracted pathways start with compartment 1 (one for particle 12, two for particle 43, and two for particle 212), as shown in Table 13.2. For these five contracted pathways, the first flow ($\rightarrow 1$) occurs at 21.2, 30.4, 65.8, 31.2, and 98.0 time units, respectively. Only the second ($\rightarrow 1 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow *$) and the fourth ($\rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 3 \rightarrow *$) contracted pathways have their first flow time in the interval $[30,\ 32]$. For the second contracted pathway, Particle 43 enters compartment 1 at 30.4 time units and visits compartment 3 twice, staying for 15.5 and 24.9 time units, respectively. For the fourth contracted pathway, Particle 212 enters compartment 1 at 31.2 time units and visits compartment 3 twice also, staying for 18.2 and 8.1 time units, respectively. Therefore:

$$S_{31}(t\ =\ 31) \approx \frac{(15.5 + 24.9) + (18.2 + 8.1)}{2}\ =\ 33.35$$

In general, we compute $S(t)$ as follows:

$$S_{ij}(t) \approx S_{ij}([t-h,\ t+h])\ \ = \frac{\sum_{p \in P_j(t-h,t+h)} \left(\begin{array}{c} \text{Sum of residence times at} \\ \text{compartment } i \text{ for pathway } p \end{array} \right)}{\left| P_j(t-h,\ t+h) \right|} \tag{5}$$

where $P_j(t-h,\ t+h)$ is a list of contracted pathways that start with compartment j. This list contains the particles that enter compartment j during the time interval $[t-h,\ t+h]$. $|P_j(t-h,\ t+h)|$ represents the number of items on this list.

We demonstrate the dynamic storage analysis computation using a simplistic lake model with three compartments: Phytoplankton (P), Zooplankton (Z), and Fish (F). The model accounts for the biomass flow among these compartments, simulating the annual changes of lake biomass. The differential equation model is as follows:

$$\begin{aligned} \dot{P} &= 1000 + 600\sin(t/8.3) - 2.5 \cdot 10^{-5} PZ - 2.5 \cdot 10^{-5} PF - 0.15P \\ \dot{Z} &= 2.5 \cdot 10^{-5} PZ - 2.5 \cdot 10^{-5} ZF - 0.1Z \\ \dot{F} &= 2.5 \cdot 10^{-5} PF + 2.5 \cdot 10^{-5} ZF - 0.08F \end{aligned} \tag{6}$$

The predatory relations among the three compartments are modeled using Lotka-Volterra type (Lotka, 1925; Volterra, 1926) predator-prey equations (Berryman, 1992). The Phytoplankton compartment gets time-varying environmental input $(1000 + 600\sin(t/8.3))$, which represents the fluctuating availability of nutrients and sunlight with seasonal variation. Figure 13.6a shows the time course of compartmental storage values. Successive peaks of storage values for the three compartments are in

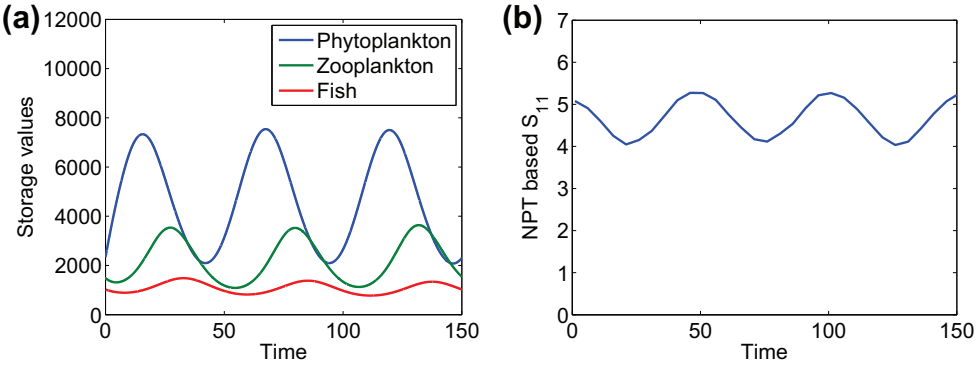

FIGURE 13.6 (a) Time course of biomass storage, simulated using the differential equations (see Eqn. (6)) for the simplistic lake model. The oscillations are indicative of the seasonal changes. (b) The first entry of the dynamic storage analysis matrix $S_{11}(t)$ computed for this model. For color version of this figure, the reader is referred to the online version of this book.

accordance with their trophic level in the lake ecosystem. Figure 13.6b shows one element of the dynamic storage analysis matrix $S(t)$, computed using $h = 10$ time units. We observe that the period of oscillations in Fig 13.6a and b coincide with each other (about 50 time units). $S_{11}(t)$ represents how much storage is generated at compartment 1 (Phytoplankton) by a unit input into itself. Comparing Figs 13.6a and b, we observe a negative correlation between S_{11} and the storage value of Phytoplankton. This is because any input received by the Phytoplankton at its lowest storage value is more likely to be retained longer as its storage value increases over time. Similarly, at its peak storage value, any input that the Phytoplankton receives is more likely to be lost as its storage value declines. This inverse relation indicates that more complicated and insightful results might be observed for larger systems with feedback cycles.

13.8 Conclusion

Individual-based studies of ecosystem flows are now within reach, thanks to sophisticated mathematical methods, efficient computational algorithms, and advances in computer technology. NPT simulations, although costly for extremely large models, provide new ways to analyze ecosystems that were not possible before.

In this chapter, we presented an individual-based methodology to compute various well-known system-wide ecological network properties. It turns out that this pathway-based methodology is simpler and more intuitive as opposed to the conventional algebraic methods based on matrix power series. The agreement of both methodologies verifies that the rather complicated algebraic formulations of the current NEA measures do accurately reflect their intended meanings. However, this new approach is not an alternative, but a parallel development to the existing methodology, extending the applicability of useful ecosystem properties to include dynamic, time-varying systems.

The fact that numerous essential research problems such as environmental impacts, climate changes, and regime shifts are centered around change increases the importance and impact of the methodology presented here.

Stochastic simulations discussed in this chapter are based on ODE models, assuming all flows leave the compartment following exponential distributions. However, this is not an accurate description of real ecosystems, since the flow material often has to have a time delay in each compartment. In other words, an input into a compartment rarely leaves that compartment immediately because biological processes such as digestion and respiration take time. For accurate representation of real models, more appropriate probability distributions (e.g., log-normal distribution) can be used instead of exponential distribution. Such changes can be easily incorporated into our stochastic models.

Another advantage of the NPT methodology is its ability to represent a wider range of scenarios than ODE or PDE models. Since NPT is an individual-based method, hybrid models where particles actually represent individual organisms, displaying intelligent behavior, combining both thermodynamical and animal behavior can be built. However, the compatibility between ODE and the NPT methodology will be broken as the ODE models do not have such flexibility.

Not everyone has quick access to NPT simulations. Therefore, simulation-based results are integrated into an experimental version of EcoNet (http://eco.engr.uga.edu), a free online software for modeling, simulation, and analysis (Kazanci, 2007, 2009; Schramski et al., 2010). This integration makes this rather computationally heavy method accessible to a wide range of scientists.

For steady-state models, the conventional methodology is still preferable because it is easier to use, simulations are not necessary, and the results are exact values. However, the conventional method only computes average behavior, whereas the NPT-based method incorporates noise and randomness, allowing the computation of standard deviation over multiple simulations. The focus of the work presented here is to provide a more capable alternative methodology still compatible with the currently available methods. For this purpose, we only use the mean of stochastic simulations. However, the additional information provided by the standard deviation and higher-order moments is an interesting topic to investigate for future studies.

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