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Throughflow analysis: A stochastic approach

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ABSTRACT

Ecological network analysis (ENA), predicated on systems theory and Leontiev input–output analysis, is a method widely used in ecology to reveal ecosystem properties. An important ecosystem property computed in ENA is throughflows, the amount of matter/energy leaving each compartment of the ecosystem. Throughflows are analyzed via a matrix **N** representing their relationships to the driving input at the boundary. Network particle tracking (NPT) builds on ENA to offer a Lagrangian particle method that describes the activity of the ecosystem at the microscopic level. This paper introduces a Lagrangian throughflow analysis methodology using NPT and shows that the NPT throughflow matrix, $\mathcal{N}$, agrees with the conventional ENA throughflow matrix, **N**, for ecosystems at steady-state with donor-controlled flows. The matrix $\mathcal{N}$ is computed solely from the pathways (particles' histories) generated by NPT simulations and its average over multiple runs of the algorithm with longer simulation time agrees with the Eulerian **N** matrix (Law of Large Numbers). While the traditional NEA throughflow analysis is mostly used with steady-state ecosystem models, the Lagrangian throughflow analysis that we propose can be used with non-steady-state models and paves the way for the development of dynamic throughflow analysis.

1. Introduction

Ecological systems modeling benefited from diverse and disparate influences. Early models (e.g., Malthus, 1798; Lotka, 1925; Volterra, 1926) were of nonlinear population processes that generally did not explicitly account for environment. Tracer experiments (e.g., Sheppard and Householder, 1951; Teorell, 1937) conducted in medical research indirectly included the environment by injecting a dye or radioactive substance to observe its pathway through the system to the point of exit. Such experiments led to the development of linear differential equations with constant coefficients, which were subsequently adopted in ecology for compartment modeling (Matis et al., 1979). The latter developed in parallel with systems ecology, which arguably arose from a need to include environment more explicitly in models describing the movement of energy and matter through different trophic (feeding) levels (Lindeman, 1991) or entire ecosystems (Odum, 1957).

A key element in compartment modeling is that the quantities transferred are conservative. Compartment models take a macroscopic control-volume, or Eulerian, perspective that groups particle activity into average stocks (compartment storages) and flows (inter-compartmental transactions). Its mathematical descriptions distinguish system (inside the control volume) from environment (outside), and dynamics proceeds from initial through transient to steady states. At steady state, inflow equals outflow at both the system level and the individual compartment level. Such states are only macroscopically "steady", however, because at the level beneath the aggregate stocks and flows, absent attainment of thermodynamic equilibrium, the individual particles making up these quantities continue in dynamic motion. A shortcoming of the Eulerian approach is that the finer level of detail that actually gives rise to the aggregate stocks and flows is impossible to study. On the other hand, an alternative Lagrangian methodology to describe each individual particle's relevant dynamics is impractical for most ecological analyses because supporting data at the particle level cannot be obtained. The problem is the same as in the distinction in physics between mechanics and statistical mechanics, suggesting a stochastic approach may also be appropriate for compartmental systems. The network particle tracking (NPT) method used in this paper is such a stochastic methodology. It describes the movement of individual particles within the system and in exchange with the environment (Tollner and Kazanci, 2007). Whereas a differential

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equation description of a system provides an aggregate accounting of storages and flows, beneath this accounting are the continuously changing motions and positions of countless (but finite) individual particles. Essentially NPT allows for a model to account for the environment's open flow characteristics where subsequently over time, this continuous stochastic activity averages to predictable or even steady-state storages and flows. In this study, by tracking apparently random individual path histories of particles in a network, we account for their histories and then show that their throughflow activity, when averaged, is actually the same as the activity calculated and represented by traditional analytic methods. We account for the system and its surrounding environment's stochastic behavior and show that this behavior, when considered in total, can actually present itself as steady-state activity.

Simulating the incremental behavior of individual particles affords an opportunity to both expand ecological network analysis (ENA) methodology and better understand microdynamic ecosystem behavior Gattie et al. (2006). For example, using current ENA methods, inputs from the environment can be readily mapped to throughflows in the system. However, NPT allows an additional resolution of internal system activity, through detailed information of individual particle activity, by revealing to what extent inputs from internal system compartments contribute to the system throughflows. NPT is also capable of simulating ecosystems evolving over time (diurnal, seasonal, long-term climate change, etc.) where model output can be used to assess dynamic, averaged, or other groupings of ecological properties. Essentially, NPT represents an ability to reveal actual system activity at different resolutions. Especially, NPT simulations reveal that all meaningful and measurable exchanges between system components over a finite time occur along pathways of bounded length. Therefore, the throughflow matrix **N** is accurately measured as a finite sum. Considering the underlying dynamic and stochastic behavior of ecosystems in general, we begin to examine the system microdynamics behind observed ecosystem activity.

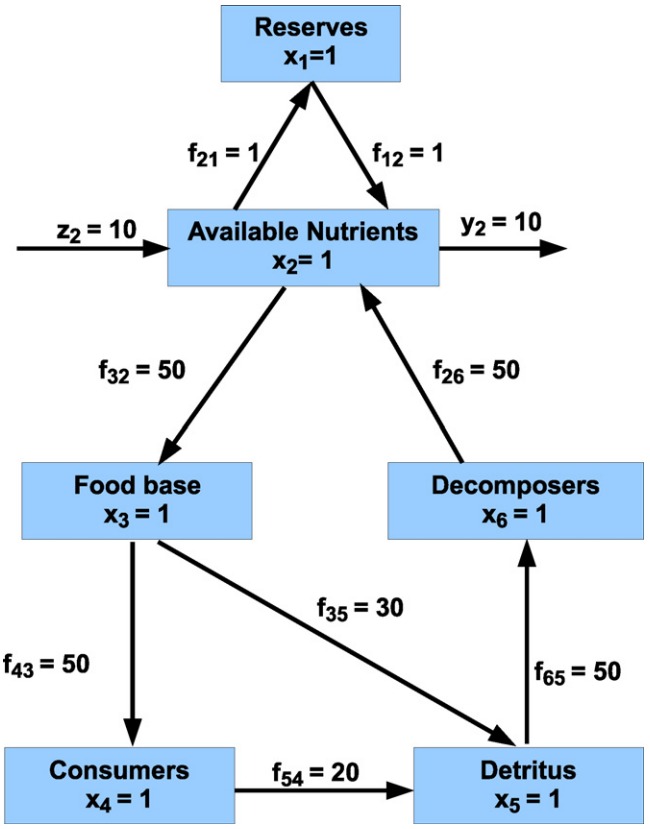

Fig. 1. An example of energy or matter flows and storages in an ecosystem model. Labels $\mathbf{x}_i$ denote the stock values of nodes i, $\mathbf{z}_i$ are the environmental input at node i, $\mathbf{y}_i$ are the output flow from node i, and $\mathbf{f}_{ij}$ is the direct flow from node j to node i inside the system.

2. Compartment models: general form

Systems ecology takes a holistic approach to study organisms by embedding them in their natural habitat and investigating their behavior as they mutually interact, directly and indirectly, with one another and also with the abiotic resource and habitat variables that define the conditions for life. The prescription "directly and indirectly" establishes that the spheres of influence within an ecosystem must be interconnecting networks of interactions, for it is these that both enable and reflect the fact that indirect relationships are important in system dynamics (Higashi and Patten, 1989). Ecological network analysis (ENA) is a mathematical methodology derived from system theory and input–output analysis. It studies individuals as part of connected networks to elucidate their role in the web of interrelationships with other components and with the surrounding environment (Patten, 1978; Fath and Patten, 1999). The main goal of ENA is to examine the interdependence of organisms in a biota and quantify the interactions, direct and indirect, between any arbitrary pair of compartments in an interconnection. Due to mathematical difficulties, the present theory is developed for steady-state systems only, although several previous initiatives have explored methods for dynamic systems (e. g., Hippe, 1983; Hallam and Antonios, 1985).

In ENA, systems are modeled as weighted digraphs (directed graphs) with tentacles. The weighted nodes correspond to compartments that store conservative quantities. Compartments can be biotic or abiotic aggregates of species, groups of species, or organic or inorganic substances, or mixtures of all such categories. Arcs, which are oriented weighted edges interconnecting the nodes, represent substance transfers between the compartments. The transfers represent conservative flows, and the tentacles are arcs connecting the interior compartments to the external environment. Realistically, due to inherent randomness of the generating processes, these functions are, or should be (they are not in conventional ENA), stochastic. With these specifications, we can proceed to identify and notate the relevant model quantities, all of which are implicitly functions of time:

$\mathbf{x}_i$	:	storage value of the modeled substance at node i.
$\mathbf{f}_{ij}$	:	flow of the modeled substance from node j to node i per unit of time.
$\mathbf{z}_i$	:	driving input from the environment to i.
$\mathbf{y}_i$	:	dissipative output to the environment at node i.
$\mathbf{T}_i^{\text{in}}$	:	throughput(sum of inflows)into node i
$\mathbf{T}_i^{\text{out}}$	:	throughflow(sum of outflows)out of node i

Fig. 1 illustrates these quantities (except the throughflows) for an example digraph.

In a deterministic framework, the rate of change of the stock values in any ecosystem with n nodes is governed by the following system of ordinary differential equations:

$$\frac{d\mathbf{x}_i}{dt} = \underbrace{\sum_{j=1}^{n}\mathbf{f}_{ij} + \mathbf{z}_i}_{\text{input into}i} \quad \underbrace{-\sum_{k=1}^{n}\mathbf{f}_{ki} - \mathbf{y}_i}_{\text{output from}i}, i = 1, \ldots, n. \tag{1}$$

The positive terms represent inflows to compartment i, $\mathbf{T}_i^{\text{in}}$, and the negative ones outflows, $\mathbf{T}_i^{\text{out}}$. It is the generation of these

throughflows that is the focus of this paper.

$$\mathbf{T}_i^{\text{in}} = \sum_{j=1}^{N} \mathbf{f}_{ij} + \mathbf{z}_i, \quad \mathbf{T}_i^{\text{out}} = \sum_{k=1}^{N} \mathbf{f}_{ki} + \mathbf{y}_i \tag{2}$$

The throughflow of compartment(node) i is

$$\mathbf{T}_i = \mathbf{T}_i^{\text{out}} = \sum_{k=1}^{n} \mathbf{f}_{ki} + \mathbf{y}_i \tag{3}$$

For an ecosystem at steady state, that is, the storage values $\mathbf{x}_i$ for all nodes do not change in time ($(\mathrm{d}\mathbf{x}_i/\mathrm{d}t) = 0$ at all times and for all nodes i in the network), the throughflow is

$$\mathbf{T}_i = \mathbf{T}_i^{\text{in}} = \mathbf{T}_i^{\text{out}}. \tag{4}$$

3. Conventional input–output throughflow analysis

Compartmental throughflow analysis quantifies substance flow from boundary inputs, $\mathbf{z}_j$, to interior compartments, $\mathbf{x}_i$, to boundary outputs, $\mathbf{y}_i$. Solving Eq. (3) for $\mathbf{z}_i$,

$$\mathbf{T}_i - \sum_{j=1}^{n} \mathbf{f}_{ij} = \mathbf{z}_i \tag{5}$$

and expressing each $\mathbf{f}_{ij}$ as a fraction of the throughflow of the donor compartment:

$$\mathbf{g}_{ij} = \frac{\mathbf{f}_{ij}}{\mathbf{T}_j} \Leftrightarrow \mathbf{f}_{ij} = \mathbf{g}_{ij}\mathbf{T}_j, \tag{6}$$

Eq. (5) becomes

$$(\mathbf{I} - \mathbf{G})\mathbf{T} = \mathbf{z}, \tag{7}$$

where $\mathbf{I}$ is the $n \times n$ identity matrix, $\mathbf{G}$ is the $n \times n$ throughflow-normalized direct flow matrix (Eq. (6)), $\mathbf{T}$ is the $n \times 1$ vector of throughflows and $\mathbf{z}$ the $n \times 1$ vector of environmental inputs.

From Eq. (7), assuming $\mathbf{I} - \mathbf{G}$ is invertible, a mapping from the boundary input vector, $\mathbf{z} = [\mathbf{z}_i]$, to the interior throughflow vector, $\mathbf{T} = [\mathbf{T}_i]$ follows:

$$\mathbf{T} = \mathbf{N}\mathbf{z} \quad \text{where} \quad \mathbf{N} = (\mathbf{I} - \mathbf{G})^{-1}. \tag{8}$$

This is standard steady-state ENA and NEA formulation for throughflow. It enables the computation of throughflows generated by a given input vector, $\mathbf{z}$, as the matrix product $\boldsymbol{Nz}$. For example, if $\mathbf{z} = [1, 0, \ldots, 0]^T$, representing one unit of substance introduced into the system at compartment 1, the corresponding throughflow generated would be

$$\begin{bmatrix} \mathbf{n}_{11} & \cdots & \mathbf{n}_{1n} \\ \vdots & \ddots & \vdots \\ \mathbf{n}_{n1} & \cdots & \mathbf{n}_{nn} \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{n}_{11} \\ \vdots \\ \mathbf{n}_{n1} \end{bmatrix}. \tag{9}$$

This quantifies the contributions made to each of the n throughflows by a unit input into compartment 1, and it follows that $\mathbf{n}_{ij}$ quantifies the amount of nutrients that move through i due to a unit of input into j.

From Markov chain theory, the coefficients $\mathbf{n}_{ij}$ also have an alternative interpretation as the number of times a unit of substance introduced at j will appear at i while it remains in the system. If the term "unit" as used in this paragraph is interpreted as a "particle", one can see how the conventional input–output methodology of ENA and NEA relates conceptually to the particle tracking methodology. Computationally, however, the two approaches are very different.

Finally, if the non-dimensional flow intensities defined in Eq. (6) satisfy for all i, $\sum_{j=1}^{n} |\mathbf{g}_{ij}| < 1$ or if the eigenvalues of $\mathbf{G}$ are all < 1, then $\mathbf{N}$ can be decomposed as follows:

$$\mathbf{N} = (\mathbf{I} - \mathbf{G})^{-1} = \mathbf{I} + \mathbf{G} + \mathbf{G}^2 + \cdots \tag{10}$$

giving for (8):

$$\mathbf{T} = \mathbf{N}\mathbf{z} = (\mathbf{I} - \mathbf{G})^{-1}\mathbf{z} = (\mathbf{I} + \mathbf{G} + \mathbf{G}^2 + \cdots)\mathbf{z} \tag{11}$$

In these expressions, $\mathbf{G}^m$ represents the m'th power of $\mathbf{G}$ whose entries, $\mathbf{g}_{ij}^{(m)}$ (parentheses signify powers obtained by matrix, not scalar, multiplication), indicate the proportion of throughflow $\mathbf{T}_j$ that reaches compartment i in m transfer steps. That is, the power series partitions $\mathbf{n}_{ij}$ into components that reach i after traveling over all pathways in the system of all possible lengths, $m = 0, 1, 2, \ldots$, leading to i from the originating compartment j. The first term, $\mathbf{I} = \mathbf{G}^0$, corresponding to $m = 0$, brings input across the boundary into the system interior (the first term, $\mathbf{I}z$, in Eq. (11)), for subsequent distribution ($\mathbf{G}z$, $\mathbf{G}^2\mathbf{z}$, $\mathbf{G}^3\mathbf{z}$, ...) over pathways of successively increasing length. The pathway aspects of the traditional approach, implicit in Eqs. (10) and (11) power series, motivate the individual-based particle tracking methodology, as next described.

4. Throughflow analysis by network particle tracking

This section presents a new approach to throughflow analysis. Recall that the main question to be answered is, for any compartmental system how much substance ($\mathbf{n}_{ij}$) does compartment i receive for each unit of that substance introduced into the system at compartment j? All ecosystems live far from steady state and continually reorganize themselves as their environment changes. However, most NEA software packages are build on the assumption that the ecosystems are at steady state (Fath and Borrett, 2006; Allesina and Bondavalli, 2004) and uses the matrix algebra approach of input–output analysis as outlined in the previous section. Using that methodology, it is not possible to evaluate the activity between two compartments under changing non-steady states. The method developed here takes a different approach, based on network particle tracking (NPT). This simulates the pathway trajectory of each particle flowing in the system during a given time period, records these histories, and then computes $\mathbf{n}_{ij}$ values simply from information contained in them. In the two subsections below, we explain first the NPT algorithm that enables labeling, tracking, and recording of individual particles during simulation of system dynamics (Section 4.1). Then, we describe how to compute a NPT-based version of $\mathbf{n}_{ij}$ utilizing information contained in the trajectories (Section 4.2). Finally, in Section 5, we compare $\mathbf{n}_{ij}$ values computed by both the conventional and NPT methods for a set of literature models.

4.1. Network particle tracking

In NPT, each unit of mass or energy is labeled and tracked in time as it flows in simulated system dynamics through the system network defined by Eq. (1). The NPT algorithm starts by partitioning initial stocks of stored substance into packets we call particles. Bookkeeping is simple: a unique integer label is assigned to each particle together with a real number representing its size as a unit of stock defined by the modeler. Next, based on flow intensities, $\mathbf{f}_{ij}$ derived from the defining equations, NPT computes which flow is next likely to occur, and when. To implement that flow, a particle is chosen at random from the donor compartment and shifted to the recipient compartment. If the chosen flow is an environmental input, then a new particle is introduced into the receiving compartment. NPT then records the trajectory of each particle as it passes through the network.

An essential property of NPT is that the simulation results are compatible with the differential equation formulation (1) of the model. In other words, the average of many NPT runs coincides with the ODE solution. Since NPT deduces its rules on how an individual particle will move directly from the ODE representation, there is no need for extra parameters or decisions, as usually is required in building individual-based models. Exact causality is preserved, whether this be linear, nonlinear, stationary, or time-varying, etc.

At steady state, the Eulerian ODE Eq. (1), gives the illusion that the system is static as no macroscopically observable change occurs over time. In fact, however, substance continues to enter and leave each compartment, and the system as a whole, at equal rates, Eq. (4)). The familiar open-system example of water standing at a fixed level in a basin with fluid coming in and draining out gives no evidence that anything dynamic is happening, that water molecules are in fact continually being introduced and exhausted. NPT enables a Lagrangian assessment of such microscopic activity, and demonstrates that although compartmental storage values may be constant the pool of substance is dynamic and undergoes continual turnover. In NPT, this is demonstrated by changing identities of the stored particles in the compartments. Particle tracking makes turnover easy to recognize.

In NPT, newly introduced particles are assigned unique tags as they enter the system flow-stream. With inflow only, the stock of particles at each node and in the system would increase during simulation, but with output the dissipated particles could eventually balance the entering ones, bringing the system macroscopically to steady state. NPT recycles the memory freed by dissipated particles and appends their pathway histories to a text file. Through extensive use of such computational innovations, the algorithm takes only a few seconds to run on modern computers for models of moderate size and connectivity. Fig. 2 shows the pathway trajectories of several selected particles in a run of Fig. 1 model.

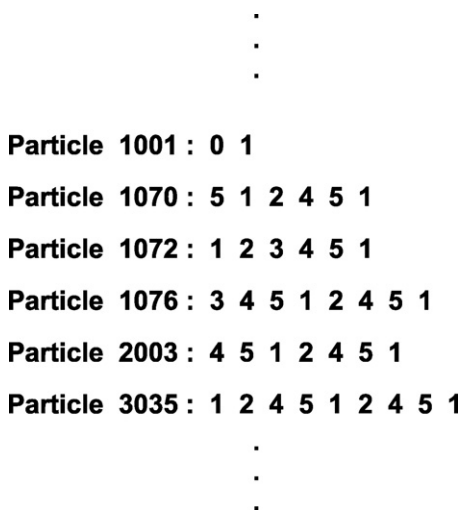

Fig. 2. Partial output from a NPT run of Fig. 1 model. Pathway trajectories of six arbitrarily selected particles are shown. Key to compartments: 0 = reserves, 1 = available nutrients, 2 = food base, 3 = consumers, 4 = detritus and 5 = decomposers.

Table 1
Example of computation of n_{ij} using a partial output of NPT.

Number of occurrences of 2 after 1	6
Number of pathways containing a 1	6
	$n_{21} \approx \frac{6}{6} = 1$
Number of occurrences of 1 in the file	12
Number of line containing a 1	6
	$n_{11} \approx \frac{12}{6} = 2$

For steady-state ecosystem models, the ODE (1) gives the illusion that the system "stopped", as nothing changes overtime. In fact, matter or energy is entering and leaving (each compartment and the system as a whole) at equal rates. NPT enables us to see the activity hidden by the ODE model (1) and demonstrates that although compartmental storage values are constant, the pool of nutrients is frequently renewed as demonstrated by the changing identities of the particles stored in compartments.

4.2. Stochastic Throughflow Analysis

The NPT algorithm uses the pathway trajectories of all the particles in a system during a simulation trial to calculate a Lagrangian version, $\mathcal{N} = (n_{ij})$ of the Eulerian throughflow matrix $\mathbf{N} = (\mathbf{n}_{ij})$, of unit-input–generated throughflows, $\mathbf{n}_{ij}$, for all (i, j) pairs of compartments. The computations are, for $j \neq i$:

$$n_{ij} = \sum_{\text{pathways}} \frac{\text{Number of occurrences of } i \text{ after } j \text{ in each pathway(any node to any node)}}{\text{Total number of paths(any node to any node)that contain } j} \tag{12}$$

and for $j = i$

$$n_{ii} = \sum_{\text{pathways}} \frac{\text{Number of occurrences of } i \text{ in each pathway(any node to any node)}}{\text{Total number of paths(any node to any node)that contain } i}. \tag{13}$$

These formulations are surprisingly simple compared to the conventional theory's (Section 3) involved rationales about direct (**G**, Eq. 10) and indirect ($\mathbf{N} - G - I$) contributions of all orders to the mapping of boundary inputs ($\mathbf{z}$) into throughflows ($\mathbf{T}$), Eq. (11). Eq. (12) says simply, for each (i, j) node pair with $i \neq j$, that the mapping of boundary input at j into interior throughflow at i is the summation, over all directed pathways in the j-to-i interconnection, of the number of times i follows j (numerator) relative to the total number of pathways that contain j (denominator). Eq. (13) gives self-influence as the summation of the number of times i occurs in all pathway trajectories, divided by the number of pathways that contain i. In the simplicity of these expressions one sees immediately how mathematical limitations of the conventional approach are obviated. The NPT method depends in no way on properties of the simulated model such as linearity, stationarity, steady state, etc. It is completely general over all classes of dynamical systems one might employ in representing ecological flow-storage networks.

As an example, let us compute n_{21} and n_{11} using the partial NPT output presented in Fig. 2. Table 1 describes this calculation, based on Eqs. (12) and (13). Repeating this calculation for all entries of $\mathcal{N}$, we get the following matrix:

$$\mathcal{N} \approx \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1.2 & 1.5 & 1.6 & 1.8 \\ 0 & 1 & 1.2 & 0.5 & 0.6 & 0.8 \\ 0 & 0.167 & 0.2 & 1 & 0 & 0 \\ 0 & 1 & 1.2 & 1.5 & 1.6 & 0.8 \\ 0 & 1 & 1.2 & 1.5 & 1.6 & 1.8 \end{bmatrix} \tag{14}$$

NPT is based on a stochastic algorithm, therefore each simulation of the same model generates a different set of pathways. However, the number of particles flowing through the system for the

same duration of simulation time will not fluctuate greatly. Therefore, computing $\mathfrak{n}_{ij}$ from the pathways recorded by NPT raises the following issues about precision and accuracy:

1. How does $\mathfrak{n}_{ij}$ vary with the number of pathways used?
2. How many pathways are needed, on average, to obtain values of $\mathfrak{n}_{ij}$ of a prescribed accuracy?
3. How does $\mathfrak{n}_{ij}$ vary over multiple simulations of the same model?

We address these questions in the next section.

5. Comparative analysis of the NPT based throughflow theory

We tested our Lagrangian throughflow theory (Section 4) by comparing the NPT based $\mathcal{N}$ and the Eulerian **N** computed for a set of 12 aquatic and terrestrial ecological models, both published and unpublished. One model, a seven-compartment description of carbon flow in an open ocean euphotic-zone ecosystem (Fasham, 1985), was used in development, and the others to demonstrate generality. Precision and accuracy of results were also considered.

5.1. Numerical Results: Development

NPT is based on a stochastic algorithm, therefore its computed $\mathcal{N}$ matrix differs for each simulation. However, the matrix converges to the conventional analytic **N** matrix (Eq. 10) as simulation time increases. To demonstrate this, we ran the Fasham (1985) model 1000 times and computed coefficient $\mathfrak{n}_{32}$ as an example. Fig. 3(a) shows the distribution of the generated values for four different simulation times. Variance of the computed $\mathfrak{n}_{32}$ values decreased to zero and the values converged to the analytic $\mathbf{n}_{32}$ value as the simulation interval was lengthened.

To determine if all entries of $\mathcal{N}$ converge to N, we define the following scalar measure of matrix discrepancy:

$$\Delta(\mathcal{N},\ \mathbf{N}) = ||\mathcal{N} - N||_\infty = \max(|\mathfrak{n}_{ij} - \mathbf{n}_{ij}|,\ 1 \le i, j \le n)$$

Note that $\Delta(\mathcal{N},\ \mathbf{N})$ is larger than any of the differences $|\mathfrak{n}_{ij} - \mathbf{n}_{ij}|$. Therefore if $\Delta(\mathcal{N},\ \mathbf{N}) = \delta$, then we have that $|\mathfrak{n}_{ij} - \mathbf{n}_{ij}| \le \delta$ for all $i, j = 1, 2, \ldots, n$.

In Fig. 3(b), $\Delta(\mathcal{N}, \mathbf{N})$ vs. simulation time is plotted for four NPT runs of the same model. In all four cases, $\Delta(\mathcal{N}, \mathbf{N})$ converges to zero as simulation time increases despite the inherent stochasticity of the NPT methodology. As $\Delta(\mathcal{N}, \mathbf{N})$ is the maximum difference, it follows that all entries of the computed stochastic simulation matrix, $\mathcal{N}$, converge to the analytic throughflow matrix, **N**.

5.2. Numerical Results: Generalization

To establish that the observed convergence in Fig. 3(b) was not specific to the chosen model, we investigated $\Delta(\mathcal{N}, \mathbf{N})$ for twelve more ecological models ranging in size from four to twelve compartments. Results are shown in Figs. 4 and 5. In every case $\mathcal{N} \to \mathbf{N}$ as simulation time increased. We conclude that the Lagrangian particle-tracking methodology of this paper (Section 4) generates, or can be made to generate with long enough simulations, comparable numerical results to those obtained with established Eulerian input–output methods (Section 3).

5.3. Numerical Results: Precision and Accuracy

Issues of precision and accuracy are germane to the NPT methodology. Here we present a few general observations about this based on our computational experience, but closer study must await future investigation.

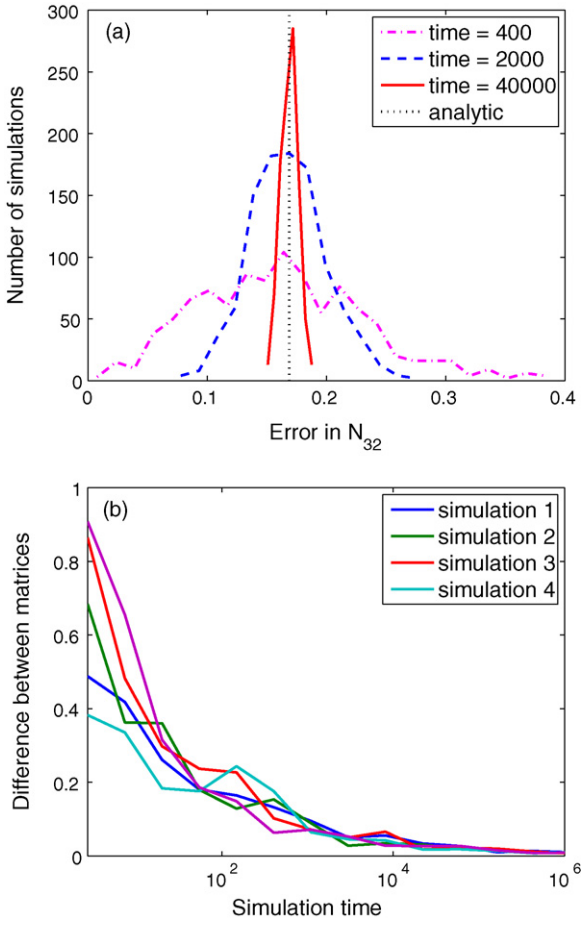

Fig. 3. Both (a) and (b) show that $\mathcal{N}$ converges to N as simulation time increases. (a) $\mathfrak{n}_{32}$ is computed using 1000 NPT simulations of the seven-compartments, euphotic open ocean, carbon flow model Fasham (1985) for four different simulation instances. (b) The scalar differences, as defined in the text, between the stochastic and conventional throughflow matrices are shown for four NPT simulation instances.

It became evident during the stochastic runs for Figs. 4 and 5 that run variances decreased as simulation time increased. This indicated that long simulation intervals are necessary to ensure sufficient precision for the purposes at hand. Similarly, as run times increased, particle pathway data continued to accumulate, producing ever closer convergence of $\mathcal{N}$ to **N**. The conclusion from this is that long run times are also needed to ensure sufficient accuracy for the desired purposes.

These observations raise a question about feasibility: how much computing time is needed to compute the NPT-based throughflow matrix precisely and accurately enough? The answer depends on the model, both size and connectivity. Our experience suggests that around 20000 particle pathways is sufficient to compute $\mathcal{N}$ to the point where the component-wise difference between $\mathcal{N}$ and **N** is less than 1%; that is, $\Delta(\mathcal{N},\ \mathbf{N}) \le \delta = 0.01$. For models of the scope and scale we used, it takes a second for NPT to generate adequate data on a modern single CPU computer.

6. Discussion

Established methods of ecological network and environ analyses (ENA, NEA) are macroscopic, deterministic and, in the main, limited to linear systems at steady state. They account for all the pathways that route substance around a system, and in this they convey the impression of parcels of material being conservatively stored and transferred over the network. The new particle-tracking

simulation (NPT) method of this paper makes these parcels explicit as particles instead of manifesting aggregate stocks and flows. It is microscopic, stochastic, and unlimited as to the kind of model or the dynamic state to which it applies. As such, it appears to significantly complement the conventional methods based on system theory and input–output analysis. Both approaches account for all pathways, direct and indirect, inherent in their defining equations. The stochastic basis of the NPT method aligns with the unpredictability of nature, and the particle focus matches the fact that the conserved quantities transferred, energy and matter, are both physically particulate at their core. The fact that two methodologies very different in concept and analytical machinery converge to give comparable numerical results from two ends of the levels-of-organization spectrum, particulate (Lagrangian) and aggregate (Eulerian), is compelling. The new theory developed here can be seen as complementing existing ENA and NEA concepts, and opening new dimensions to further understanding of ecologically important stock-and-flow networks.

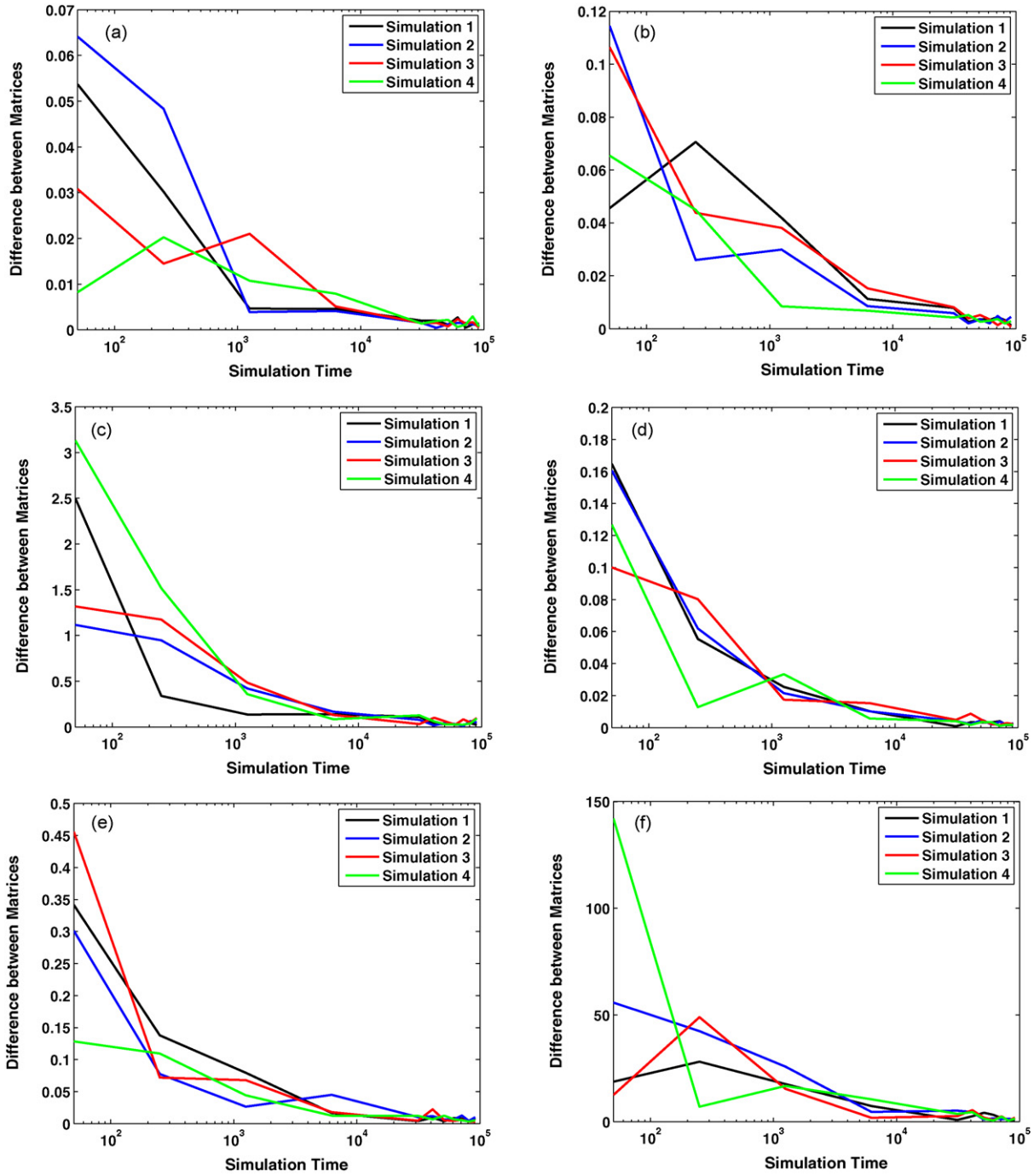

Fig. 4. Analysis of the Lagrangian throughflow matrix vs. the Eulerian input–output throughflow matrix for six models. (a) A four-compartment model of calcium flow in a tropical rain forest ecosystem, El verde National Forest, Puerto-Rico, (Jordan et al., 1972). (b) A five-compartment model of nitrogen flow in a tropical rain forest ecosystem, El Verde National Forest, Puerto-Rico, (Edmisten, 1970). (c) A generic six-compartment model of mineral flow in a temperate forest ecosystem, composite of literature data, (Webster et al., 1975). (d) A generic six-compartment freshwater lake ecosystem model, composite of literature data, (Webster et al., 1975). (e) A six-compartment model of nitrogen flow in a pine forest ecosystem, Aiken, South Carolina, USA. (f) A generic six-compartment grassland ecosystem model, composite of literature data, (Webster et al., 1975).

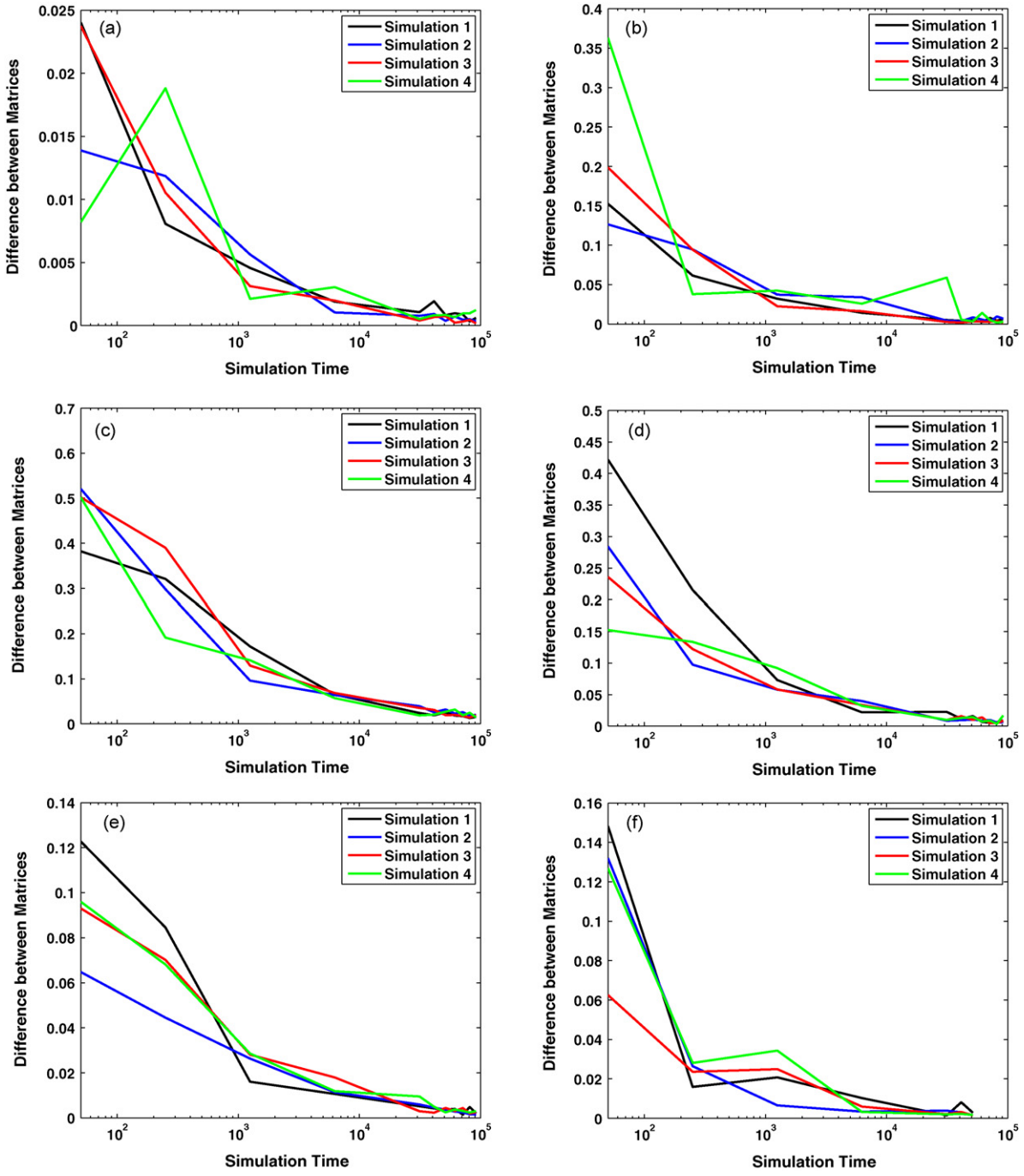

Fig. 5. Analysis of the Lagrangian throughflow matrix vs. the Eulerian input–output throughflow matrix for six more models. (a) Model of coprophagic web in chesapeake oysters community, (Haven and Morales-Alamo., 1966). (b) Model of mineral flow in a generic euphotic oceanic ecosystem,(Webster et al., 1975). (c) Open ocean mixed layer ecosystem, composite of literature data, (Hobbie, 1984). (d) A seven-compartment, euphotic open-ocean, carbon flow model, (Fasham, 1985). (e) A nine-compartment model of energy flow in the cedar bog lake ecosystem, (Lindeman, 1991). (f) Twelve-compartment chesapeake bay mesohaline ecosystem, Maryland, unpublished data, Chesapeake Biological Laboratory, Solomons, Maryland.

Simulation-based throughflow analysis has several advantages. One mentioned in the text and above is that the investigated model need not be linear, or at steady state. These have been important limitations to prior methods. NPT is capable of simulating ODE models of any mathematical form, and based on this $\mathcal{N}$ can be computed for systems that change on both short (diurnal, seasonal) and long (geologic) time scales. It seems feasible, as has been done in several ways for $\mathbf{N}$ in the conventional approach (Whipple et al., 2007), to compute $\mathcal{N}$ over a time window and advance this window stepwise to obtain a discrete approximation to a dynamic throughflow analysis.

Another point pertaining to the dynamics of natural systems is that input-to-throughflow mappings in these occur over finite pathways. Real systems do not remain constant long enough for pathways reflected in the infinite sums of matrix methodology (10) to be expressed. The requirement of running power series to infinity to obtain $\mathbf{N} = (\mathbf{I} - \mathbf{G})^{-1}$ might therefore inflate the amount of material exchanged between the compartments. Since the particle-tracking algorithm simulates real-time substance flow, it offers a way potentially to evaluate truer activity of the system over time. Three caveats apply here, however. First, after particle pathways have been generated in the NPT method, $\mathcal{N}$ is computed as in Eqs.

(13) and (12) and must be applied the input vector in the same way that **N** is in Eq. (8), that is,

$$T = \mathcal{N}\mathbf{z}. \quad (15)$$

Second, as shown in Figs. 3–5, $\mathcal{N}$ converges to **N** as the duration of simulation increases. Short NPT run times would entail similar errors in $\mathcal{N}$ to those induced in **N** by any truncation of the contributing infinite series (10). Third, the NPT methodology is no exception in having built-in errors that must be addressed and understood for correct usage.

In conclusion, NPT simulation of individual particle movements in networks affords an opportunity to both expand methodology and broaden understanding of the interplay between micro- and macrodynamics (Gattie et al., 2006). Particle tracking allows additional resolution of internal activity, and although Lagrangian approaches typically require large computational resources, these can be lessened by sophisticated mathematical innovations, efficient computational algorithms, and modern computing power itself. In Sections 4.1 and 5.3 it was observed that NPT took several seconds of computer time to run small models. With large models, such as already exist in many environmental and biomedical applications, computational expense can become limiting. Therefore, we see no need at present to curtail steady-state studies employing standard methods. Such methods may have limited descriptive power but they have great heuristic power, and are already facilitated by readily available software and software packages. The latter includes NETWRK (Ulanowicz and Kay, 1991, http://www.glerl.noaa.gov/EcoNetwrk/), Ecopath with ecosim (Christensen and Walters, 2004; http://www.ecopath.org/), WAND (Allesina and Bondavalli, 2004), a Matlab NEA function (Fath and Borrett, 2006) and EcoNet (Kazanci, 2007, http://eco.engr.uga.edu/). The evident complementarity of bi-level study is a strong reason to continue both lines of development.

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