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Network environ theory, simulation, and EcoNet® 2.0

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ABSTRACT

We introduce and codify the mathematics of Ecological Network Analysis (ENA) in general and Network Environ Analysis (NEA) in particular used by the web-based simulation software EcoNet® 2.0. Where ecosystem complexity continues to drive an increasingly vast environmental modeling effort, ENA and NEA represent maturation, in part, of the compartment modeling approach. Compartment modeling mathematically represents compartment storages with both internal-connecting and external-environmental flows as ordinary differential equations. ENA and NEA expand these mathematics into complex systems analysis and corresponding network theory. EcoNet was developed to facilitate the mathematical modeling, to enhance the overall presentation, and to improve the subsequent long-term progress of ENA and NEA systems analysis. Thus, as a continuing enhancement to the overall understanding, but more importantly, to the future growth of environmental modeling associated with ENA and NEA, we derive and summarize the canonical mathematics of ENA, NEA, and EcoNet, which facilitates their future use.

Software availability

EcoNet: Modeling, simulation, and analysis software for ecological networks and compartmental models
Contact address: Driftmier Engineering Center, University of Georgia, 597 D. W. Brooks dr., Athens, GA 30602, USA. Tel: +1 706 5420863; fax: +1 706 5428806
Year first available: 2006
Hardware required: Any device (PC, net-book, tablet, smart-phone) with a full-featured browser
Software required: Browser. EcoNet is tested on Firefox 3.5 on MS Windows, Mac OS, and Linux. EcoNet is known to work with other browsers (Internet Explorer, Chrome, Android native browser) as well
Programming language: C++, Linux shell scripts, CGI
Program size: N/A
Availability and cost: Freely accessible through the EcoNet web interface at http://eco.engr.uga.edu
Maintenance: EcoNet is regularly updated. Users have immediate access to the latest version through its web interface.

1. Introduction

Ecosystem complexity continues to drive an increasingly vast environmental modeling effort and corresponding complex systems analysis. Ecological Network Analysis (ENA) in particular represents a maturation, in part, of the previously more general compartment modeling approach (Matis et al., 1979; Walter and Contreras 1999) which pictorially and mathematically (usually linear constant coefficient differential equations) based its representation of systems of matter or energy as multiple compartments (storages, objects, etc.) and their associated connections (flows, edges, links, etc.) between themselves and with an external environment. ENA expands this multi-compartment modeling perspective into ecological systems analysis and theory (e.g., Embodied Energy Analysis—Herendeen, 1981, 1989; Network Environ Analysis—Patten, 1978, 1981, 1982, 1985; Fath and Patten, 1999; Input–Output Analysis—Hannon, 1973, 1985; and Ascendency Analysis—Ulanowicz, 1980, 1986, 1997). Examples of the available supporting software for ENA include NETWRK (Ulanowicz and Kay, 1991), ECOPATH (Christensen and Pauly, 1992), WAND (Allesina and Bondavalli, 2004), the MATLAB® script engineered by Fath and Borrett (2006), and EcoNet (Kazanci, 2007).

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1.1. EcoNet

Augmenting ENA's ongoing algorithm and software development, EcoNet is a dynamic web-based simulation and network analysis software capable of deterministic or stochastic dynamic simulation from given initial conditions for systems expressed as a set of compartments and corresponding flows. Subsequently EcoNet also performs Ecological Network Analysis using the methods primarily derived from Network Environ Analysis (NEA) on systems that reach steady-state. Running on its own server at http://eco.engr.uga.edu (requiring no installation) users can utilize EcoNet remotely through its web interface for dynamic simulation and disregard the NEA results or enter a steady-state model and use the software for steady-state Network Environ Analysis. Launched online July 2006, EcoNet's numerical engine was initially developed at Carnegie Mellon University to analyze statistical properties of large biochemical networks (>10,000 molecules). The numerical engine of EcoNet is fast and efficient, and is capable of handling non-linear models containing up to 10^5 compartments and 10^5 flows. Besides deterministic methods, EcoNet features efficient stochastic simulation algorithms based on the Langevin equation (Gillespie, 2000) and Gillespie's Stochastic Algorithm (Gillespie, 1977). The online presentation of the software purposely utilizes a simple and flexible user interface to improve access and usability (Kazanci, 2009). However, the underlying equation development for NEA in general and EcoNet in particular can vary based on the user's order of introduction of various assumptions, definitions, and algebraic manipulations. Improving clarity and consistency, we start from a typical conservation equation and the definition of throughflow to present an orderly technical description of EcoNet's equation development (Schramski, 2006; Schramski et al., 2009). The prolific and expanding use of EcoNet (over 2000 unique users from over 80 countries as of October 2009) coupled with a clear presentation and availability of the underlying equations will enhance Ecological Network Analysis in general and Network Environ Analysis in particular. Four functional analyses and a structural analysis, all in the context of NEA, are developed and or presented in Sections 2 and 3. EcoNet's organization and outputs then easily follow in Section 4.

1.2. Network Environ Analysis

NEA is a well documented systems analysis methodology succinctly introduced here as a system perspective representing every object as existing within a system of two environments defined as input-oriented and output-oriented environs (refer to Patten (1978, 1981, 1982) and Fath and Patten (1999) for a more comprehensive introduction). The object (or in the current presentation, the compartment) is a partition of two mutually exclusive halves, identified as an inflow and an outflow, wherein each direction includes an independent intersystem flow network originating or terminating at the system boundary. This particular bi-directional system view affords distinct mathematical advantages. Flows originating at the system boundary, z_i, are the focus of efferent or time-forward analysis as they subsequently proceed through the interior network. Separately, flows exiting the system boundary, y_i, are the focus of afferent or time-backward analysis through their previous paths and system manifestations back within the interior network.

2. Functional analysis

NEA utilizes four functional analyses labeled throughflow (Section 2.1), storage (Section 2.2), utility (Section 2.3), and control (Section 2.4) to illuminate network system characteristics. The equation development and subsequent analysis below for storage, utility, and control is unique to the dual environment perspective of NEA. However, the throughflow equations and analysis are broadly applicable to other input–output ENA methods.

2.1. Throughflow analysis

Throughflow analysis forms the basis of all subsequent functional NEA analyses and is comprised of the law of conservation, the definition of throughflow, convenient definitions to aid algebra and interpretation, and a consistent compartment model description throughout equation development.

2.1.1. Law of conservation

The first of two fundamental precepts of network analysis is the law of conservation often expressed using conserved mass as:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \sum_{\text{in}} \dot{m} + \sum_{\text{out}} \dot{m} \tag{1}$$

where $\dot{m}$ is the conventional nomenclature for mass flow rate. A similar equation can be written for conserved energy. The generic premise, whether mass or energy, of the ordinary differential equation (1) states that unsteady accumulation $\mathrm{d}m/\mathrm{d}t$ is equal to the sum of the total flow rate entering the space $\sum_{\text{in}} \dot{m}$ minus the sum of the total flow rate leaving $\sum_{\text{out}} \dot{m}$.

Fig. 1 shows a typical compartment within a multi-compartment model where storage, either mass or energy, is generically denoted with the letter x and intercompartmental mass or energy flow quantities are denoted with the letter f. Using this convention, Eq. (1) for an n-compartment system is the typical network compartment conservation equation,

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \sum_{\substack{j=1 \\ \text{in}}}^{n} f_{ij} + z_i - \sum_{\substack{h=1 \\ \text{out}}}^{n} f_{hi} - y_i, \quad i = 1, 2, \ldots, n \tag{2}$$

where the flow f represents a non-negative intercompartmental flow, z an input boundary flow (environmental input), and y an output boundary flow (environmental output) (Barber et al., 1979; Schramski et al., 2009). All terms can be time dependent and f_{ii} represents flow from a compartment to itself (e.g., cannibalism). Strictly interpreting equation (2), all intercompartmental flows, f_{ij} in, or f_{hi} out, (including self-flows f_{ii}) and all boundary flows z_i or y_i, participate in the compartment storage x_i rates of change by helping to add $\mathrm{d}x_i/\mathrm{d}t > 0$, subtract $\mathrm{d}x_i/\mathrm{d}t < 0$, or hold steady $\mathrm{d}x_i/\mathrm{d}t = 0$, each compartment's storage. Although ecological network analysis makes significant use of steady-state conditions $\mathrm{d}x_i/\mathrm{d}t = 0$, often dynamic analysis is an important identifier of system activity, stability, balance, function, and performance where the change in storage in compartment x_i is governed by (2). Transient analysis of compartmental network systems is

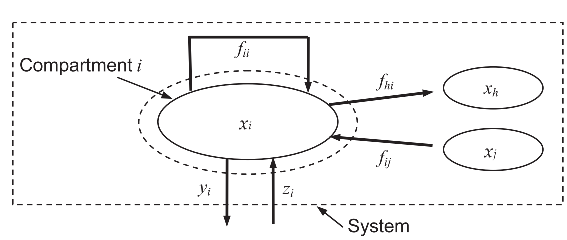

Fig. 1. Typical model compartment i within an n-compartment system, $i = 1, 2, \ldots, n$, depicting its mass or energy storage, x_i; intercompartmental flows into i, f_{ij}; intercompartmental flows out of i, f_{hi}; input boundary flow, z_i; and output boundary flow, y_i. Compartments j and h represent the rest of the compartments in the system, where $j = h = 1, 2, \ldots, n$; $j \neq i$; $h \neq i$. By convention, flow f_{ij} is from j to i and f_{hi} is from i to h.

completed by defining the initial storage of each compartment, $x(0)$, and then tracking time-forward progress through any one of several numerical methods (e.g., fourth order Runge–Kutta, Gillespie's algorithm, Runge–Kutta–Fehlberg, etc.).

2.1.2. Definition of throughflow

A compartment's storage and interactive flows, in a multi-compartment system, represent quantifiable activities or performance indices. One such index, *compartment throughflow* T_i, is a key network property, serves as an indicator of a compartment's activity within a system, and is the second fundamental precept of network analysis. Referring to Fig. 1, throughflow is defined as the sum of all flows in or out of compartment i in an n-compartment system,

$$T_i^{\text{in}} \equiv z_i + \sum_{j=1}^{n} f_{ij}, \quad i = 1, 2, \ldots, n \tag{3}$$

$$T_i^{\text{out}} \equiv y_i + \sum_{h=1}^{n} f_{hi}, \quad i = 1, 2, \ldots, n \tag{4}$$

where T_i^{in} or T_i^{out} can be unequal and are related to compartment storage accumulation,

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = T_i^{\text{in}} - T_i^{\text{out}}, \quad i = 1, 2, \ldots, n \tag{5}$$

Throughflow is a property of both the whole system and each individual compartment where *total system throughflow* (TST) is defined as the sum of all compartment throughflows,

$$\text{TST}^{\text{in}} \equiv \sum_{i=1}^{n} T_i^{\text{in}} \tag{6}$$

$$\text{TST}^{\text{out}} \equiv \sum_{i=1}^{n} T_i^{\text{out}} \tag{7}$$

whose directional values TST^{in} and TST^{out} are different in an unsteady system. Total system storage, TSS, is defined by substituting (6) and (7) into (5),

$$\frac{\mathrm{dTSS}}{\mathrm{d}t} \equiv \text{TST}^{\text{in}} - \text{TST}^{\text{out}} \tag{8}$$

For a steady-state system where all compartment and total system storages remain constant, $\mathrm{d}x_i/\mathrm{d}t = 0$ and $\mathrm{dTSS}/\mathrm{d}t = 0$, Eqs. (5) and (8) reduce to,

$$T_i = T_i^{\text{out}} = T_i^{\text{in}}, \quad i = 1, 2, \ldots, n \tag{9}$$

$$\text{TST} = \text{TST}^{\text{out}} = \text{TST}^{\text{in}} \tag{10}$$

Computationally, at steady-state the directionality of throughflows becomes moot by the equalities in (9) and (10). Algebraically however, for steady and unsteady systems, a throughflow's directional orientation in Eqs. (9) and (10) is one of the fundamental constructs of input–output analysis (Leontief, 1936, 1966; Hannon, 1973; Patten, 1978) and is uniquely fundamental to Network Environ Analysis's (NEA's) mutually distinct and directional input and output-oriented environs (Patten, 1978, 1981, 1982, 1985; Fath and Patten, 1999). Throughflows are by definition [Eqs. (3), (4), (6), and (7)] enfolded composite flows with input and output boundary flows and directional intercompartmental flows as constituents. Although throughflows can be a key system representation of network activity, they can also be further parsed into their respective constituents of directional boundary (z_i or y_i) and intercompartmental partitioned microdynamic flows revealing additional compartment and network characteristics (Gattie et al., 2006a, b).

2.1.3. Time-forward: **N** matrix

The efferent or time-forward equations are developed by combining the outward oriented throughflow equation (4) for T_i^{out} with conservation equation (2) (Barber et al., 1979),

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \sum_{\substack{j=1 \\ \text{in}}}^{n} f_{ij} + z_i - T_i^{\text{out}}, \quad i = 1, 2, \ldots, n \tag{11}$$

At steady-state, $\mathrm{d}x_i/\mathrm{d}t = 0$, Eq. (11) reduces to,

$$T_i^{\text{out}} = \sum_{\substack{j=1 \\ \text{in}}}^{n} f_{ij} + z_i, \quad i = 1, 2, \ldots, n \tag{12}$$

where the right-hand side T_i^{in} is defined in (3). In matrix form (12) is,

$$\mathbf{T}_{n\times 1}^{\text{out}} = \mathbf{F}_{n\times n}[1]_{n\times 1} + \mathbf{z}_{n\times 1} \tag{13}$$

where $\mathbf{F} \equiv [f_{ij}]$ is defined as the intercompartmental flow matrix and $[1]_{n\times 1}$ is a vector of ones. Equations (11) and (12) depict incoming throughflow T_i^{in} as the sum of incoming intercompartmental flows f_{ij} and the incoming boundary flow z_i which drive future ($t_0 \le t < \infty$) behavior of the system T_i^{out}. The input–output dual perspective of environ analysis (Patten, 1978; Fath and Patten, 1999) interprets intercompartmental flows f_{ij} simultaneously as an outflow from j or inflow to i. Taking f_{ij} in the output from j orientation, a corresponding flow intensity g is defined as a function of the output throughflow of j,

$$g_{ij} \equiv \frac{f_{ij}}{T_j^{\text{out}}} \tag{14}$$

Here, g_{ij} is the fraction (dimensionless) of output throughflow at donor component j contributed to the focal component i. Rearranging (14) and substituting into (11) yields:

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \sum_{\substack{j=1 \\ \text{in}}}^{n} g_{ij} T_j^{\text{out}} + z_i - T_i^{\text{out}}, \quad i = 1, 2, \ldots, n \tag{15}$$

and at steady-state,

$$T_i^{\text{out}} = \sum_{\substack{j=1 \\ \text{in}}}^{n} g_{ij} T_j^{\text{out}} + z_i, \quad i = 1, 2, \ldots, n \tag{16}$$

For continuity and completeness, a brief review of NEA theory follows. Considering the steady-state case to aid subsequent algebra, (16) is written in matrix form for an n-compartment system as,

$$\mathbf{T}_{n\times 1}^{\text{out}} = \mathbf{G}_{n\times n}\mathbf{T}_{n\times 1}^{\text{out}} + \mathbf{z}_{n\times 1} \tag{17}$$

Solve for $\mathbf{T}_{n\times 1}^{\text{out}}$:

$$\mathbf{T}_{n\times 1}^{\text{out}} = [\mathbf{I}_{n\times n} - \mathbf{G}_{n\times n}]^{-1}\mathbf{z}_{n\times 1} \tag{18}$$

where $\mathbf{I}$, the identity matrix, is dimensionless. The identity matrix is an $n \times n$ square matrix with ones on the main diagonal and zeros elsewhere. For convenience, the term $[\mathbf{I}_{n\times n} - \mathbf{G}_{n\times n}]^{-1}$ is redefined as,

$$\mathbf{N}_{n\times n} \equiv [\mathbf{I}_{n\times n} - \mathbf{G}_{n\times n}]^{-1} \tag{19}$$

such that (18) is generally written,

$$\mathbf{T}^{\text{out}}_{n\times 1} = \mathbf{N}_{n\times n}\mathbf{z}_{n\times 1} \tag{20}$$

Hannon (1973) referred to the individual n_{ij} coefficients as structural elements of the ecosystem since $\boldsymbol{z}$ can be varied to produce changes in $\mathbf{T}$ without changing $\mathbf{N}$. $\mathbf{N}$ acts as a steady-state transfer function, taking system boundary inputs $\mathbf{z}_{n\times 1}$ through to their interior throughflows $\mathbf{T}^{\text{out}}_{n\times 1}$. Each coefficient n_{ij} represents the amount of throughflow generated at compartment i by a unit input to compartment j. The mapping matrix $\mathbf{N}$ is also known as an integral flow matrix because it accounts for all direct and indirect flows between each interior compartment (Patten, 1978; Fath and Patten, 1999; Gattie et al., 2006a, b) over all paths of all lengths. $\mathbf{N}$ can be decomposed by path length m into an infinite series (Ore, 1962),

$$\mathbf{N} = [\mathbf{I} - \mathbf{G}]^{-1} = \mathbf{G}^0 + \mathbf{G}^1 + \mathbf{G}^2 + \mathbf{G}^3 + \cdots + \mathbf{G}^m = \sum_{m=0}^{\infty} \mathbf{G}^m \tag{21}$$

This series partitions input-to-throughflow mapping coefficients into contributions from paths of each length m carrying substance from the system boundary to interior compartments. The ecological significance of Eq. (21) cannot be over stated. The convergent power series confers and confirms potentially infinite connectivity of indirect relationships between all compartments of a system with well-connected graphs of transactions. This is central to the premise that indirect effects can dominate the activities of a system (Patten, 1983; Higashi and Patten, 1986, 1989). Moreover, output-oriented environs are implicit in the $\mathbf{N}$ matrix. Each compartment's time-forward connectivity, in a multi-compartment system, subsequently maps this boundary flow forward in time through its output environ-oriented flows entailing all direct and indirect pathways m, of all lengths $m \to \infty$. Very similar in scope to time-forward throughflow equation development, the following Section 2.1.4 is an abbreviated presentation of afferent or time-backward steady-state throughflow equation development.

2.1.4. Time-backward: $\boldsymbol{N'}$ matrix

Combine equations (2) and (3),

$$\frac{dx_i}{dt} = T_i^{\text{in}} - \sum_{\substack{h=1 \\ \text{out}}}^{n} f_{hi} + y_i, \quad i = 1, 2, \ldots, n \tag{22}$$

for steady-state,

$$T_i^{\text{in}} = \sum_{\substack{h=1 \\ \text{out}}}^{n} f_{hi} + y_i, \quad i = 1, 2, \ldots, n \tag{23}$$

where the right-hand side T_i^{out} is defined in Eq. (4). Equations (22) and (23) depict outgoing throughflow T_i^{out} as the sum of outgoing intercompartmental flows f_{hi} and boundary flow y_i driven by past $(-\infty < t \leq t_0)$ behavior of the system, T_i^{in}. Recall $T_i^{\text{in}} = T_i^{\text{out}}$ at steady-state. Each empirical flow f_{hi} is both an outflow from i and inflow to h. Non-dimensional g' is defined by orienting the perspective of f_{hi} as inflow to h where the corresponding flow intensity g' is defined as a function of the input throughflow of h,

$$g'_{hi} \equiv \frac{f_{hi}}{T_h^{\text{in}}} \tag{24}$$

Rearrange and substitute into (22):

$$\frac{dx_i}{dt} = T_i^{\text{in}} - \sum_{\substack{h=1 \\ \text{out}}}^{n} g'_{hi} T_h^{\text{in}} + y_i, \quad i = 1, 2, \ldots, n \tag{25}$$

for steady-state,

$$T_i^{\text{in}} = \sum_{\substack{h=1 \\ \text{out}}}^{n} g'_{hi} T_h^{\text{in}} + y_i, \quad i = 1, 2, \ldots, 3 \tag{26}$$

In matrix form to aid algebra:

$$\mathbf{T}^{\text{in}}_{1\times n} = \mathbf{T}^{\text{in}}_{1\times n}\mathbf{G}'_{n\times n} + \mathbf{y}_{1\times n} \tag{27}$$

Rearrange:

$$\mathbf{T}^{\text{in}}_{1\times n} = \mathbf{y}_{1\times n}[\mathbf{I}_{n\times n} - \mathbf{G}'_{n\times n}]^{-1} \tag{28}$$

Define:

$$\mathbf{N}'_{n\times n} \equiv [\mathbf{I}_{n\times n} - \mathbf{G}'_{n\times n}]^{-1} \tag{29}$$

Substitute (29) into (28):

$$\mathbf{T}^{\text{in}}_{1\times n} = \mathbf{y}_{i\times n}\mathbf{N}'_{n\times n} \tag{30}$$

Eq. (30) corresponds to Leontief's (1936) original input–output analysis relationship wherein economic activity upstream necessary to produce an industrial output, y, could be determined and evaluated. Patten's afferent input-oriented environs are implicit in the $\boldsymbol{N'}$ matrix of (30). Each coefficient n'_{ij} represents the amount of throughflow generated at compartment j for a unit of boundary (environmental) output at compartment i. Compartment outputs $\mathbf{y}$ can be mapped backwards through these input environs containing all the direct and indirect pathways of all lengths [i.e., as $m \to \infty$; reference equation (31)], to incoming compartment throughflows, $\boldsymbol{T}^{in}$. Similar to Eq. (21), $\boldsymbol{N'}$ can be written:

$$\mathbf{N}' = \left[\mathbf{I} - \mathbf{G}'\right]^{-1} = \mathbf{G}'^0 + \mathbf{G}'^1 + \mathbf{G}'^2 + \mathbf{G}'^3 + \cdots + \mathbf{G}'^m = \sum_{m=0}^{\infty} \mathbf{G}'^m \tag{31}$$

The integral flow matrix $\mathbf{N}'$ is the summation of the infinite power series of $\mathbf{G}'$ which represents the partitioning coefficients for mapping boundary output $\mathbf{y}_i$ at any compartment i into flows to i from the remaining compartments in the system along all pathways of all lengths, m. Each compartment's afferent connectivity establishes first a reference to the outside system through the output boundary flow $\boldsymbol{y}$ and then subsequently maps this boundary flow backwards in time through its input-oriented environ flows over all direct and indirect pathways, m, of all lengths (i.e., $m \to \infty$).

2.2. Storage analysis

Steady-state storage analysis reformulates steady-state throughflow analysis by introducing compartment turnover rates ρ_i and storages x_i to the throughflow modeling equations.

2.2.1. Time-forward: $\boldsymbol{S}$ matrix

By definition, the total compartment's donor-specific turnover rate (units of reciprocal time, T^{-1}) is:

$$\rho_i \equiv \frac{T_i^{\text{out}}}{x_i}, \quad i = 1, 2, \ldots, n \tag{32}$$

where T_i^{out} is the total steady-state throughflow out of donor compartment i and x_i is the total steady-state storage at donor compartment i. The reciprocal of ρ_i is turnover time τ_i, also called compartment storage residence time. Turnover rates are partitioned by intercompartmental flows f_{ij} which contribute to the total compartment turnover rate. As such, for a compartment j, the donor controlled, output-oriented *partial turnover rate* is:

$$\widehat{\rho}_{ij} \equiv \frac{f_{ij}}{x_j} \quad j = 1,2,\ldots,n; \; i = 1,2,\ldots,n \tag{33}$$

where f_{ij} is steady-state intercompartmental flow from the donor compartment j to the receiver compartment i and x_j is the donor compartment j storage. The partial turnover rate $\widehat{\rho}_{ij}$ represents intercompartmental flow f_{ij} from j specifically oriented towards i contributing to overall storage turnover of compartment j. As such these partial turnover rates form the basis of a stock-oriented description of the intercompartmental flow matrix, **F**. The reciprocal of partial turnover rate $\widehat{\rho}_{ij}$ is partial turnover time $\widehat{\tau}_{ij}$ which represents compartment j's storage turnover time attributed specifically to the partitioned intercompartmental flow from compartment j directed towards compartment i. The individual partitioned turnover rates combine to equal a total compartment turnover rate,

$$\rho_j = \sum_{i=1}^{n} \widehat{\rho}_{ij} + \frac{y_j}{x_j} \quad j = 1,2,\ldots,n; \; i = 1,2,\ldots,n \tag{34}$$

expressed as donor specific partitioned turnover rates from both intercompartmental and boundary flows for compartment j.

Throughflows and intercompartmental flows are first expressed as products of the compartment storages and corresponding total and partial turnover rates,

$$T_i^{\text{out}} = \rho_i x_i, \quad i = 1,2,\ldots,n \tag{35}$$

$$f_{ij} = \widehat{\rho}_{ij} x_j, \quad j = 1,2,\ldots,n, \; i = 1,2,\ldots,n \tag{36}$$

Substituting (35) and (36) into (12) reformulates the linear throughflow model into fractions of donor compartment turnover:

$$\rho_i x_i = \sum_{j=1}^{n} \widehat{\rho}_{ij} x_j + z_i, \quad i = 1,2,\ldots,n \tag{37}$$

Expressed in matrix form:

$$\begin{bmatrix} \rho_1 & 0 & \cdots & 0 \\ 0 & \rho_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \rho_n \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \widehat{\rho}_{11} & \widehat{\rho}_{12} & \cdots & \widehat{\rho}_{1n} \\ \widehat{\rho}_{21} & \widehat{\rho}_{22} & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \widehat{\rho}_{n1} & \cdots & \cdots & \widehat{\rho}_{nn} \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} \tag{38}$$

combining similar terms,

$$\begin{bmatrix} \left(\rho_1 - \widehat{\rho}_{11}\right) & -\widehat{\rho}_{12} & \cdots & -\widehat{\rho}_{1n} \\ -\widehat{\rho}_{21} & \left(\rho_2 - \widehat{\rho}_{22}\right) & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ -\widehat{\rho}_{n1} & \cdots & \cdots & \left(\rho_n - \widehat{\rho}_{nn}\right) \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} \tag{39}$$

where the composite **C**, comprised of donor controlled, output-oriented, partial turnover rates joined with total turnover rates on the diagonal is then defined,

$$[\mathbf{C}] \equiv \begin{bmatrix} -\left(\rho_1 - \widehat{\rho}_{11}\right) & \widehat{\rho}_{12} & \cdots & \widehat{\rho}_{1n} \\ \widehat{\rho}_{21} & -\left(\rho_2 - \widehat{\rho}_{22}\right) & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \widehat{\rho}_{n1} & \cdots & \cdots & -\left(\rho_n - \widehat{\rho}_{nn}\right) \end{bmatrix} \tag{40}$$

The turnover rates in **C** can also be called rate coefficients (Patten class notes), donor controlled flow coefficients (Kazanci, 2009), or transfer coefficients (Matis and Patten, 1981) if we consider them to be donor flow-rate coefficients in the sense that model flow rates are a function of the storage level of the donor compartments (a.k.a., donor control). If the self-flow terms f_{ii} are zero, the corresponding partial rate coefficients are zero, $\widehat{\rho}_{ii} = 0$. The diagonals of (38), (39), and (40) would then solely be defined by the compartment throughflow as shown in (32). However, if $f_{ii} \neq 0$ such as with Odum's (1957) Silver Spring model, the definition of **C** in (40) is still capable of carrying the self-flow empirical data through subsequent network analysis.

Pursuing a storage transfer decomposition [corresponding convergent series format similar to Eqs. (21) and (31)], first a non-dimensional ***P*** is defined for convenience,

$$\mathbf{P}_{n\times n} \equiv \mathbf{I}_{n\times n} + \mathbf{C}_{n\times n}\Delta t \tag{41}$$

where **I** is the identity matrix. By definition, **P** is constructed of both **C** and **I**. The **P** matrix is a uniquely revealing construct of information regarding the storage turnover relationships between compartments. The off diagonal elements of the **P** matrix, p_{ij}, represent fractions of storage x_j in compartment j transferred to storage at i, x_i, during the interval t to $t+\Delta t$. The diagonal terms, p_{ii}, are different due to the algebraic definition generating the composite **P** matrix. The diagonal terms identify the fraction of the original quantity of mass or energy remaining in each compartment after the discrete time step Δt. Recall the system is assumed at steady-state. As mass or energy leaves a compartment's storage, an equal amount replaces it. Total storage content x_i remains constant. Substitute the definition of **C** into (39),

$$-\mathbf{C}_{n\times n}\mathbf{x}_{n\times 1} = \mathbf{z}_{n\times 1} \tag{42}$$

and multiply by a ratio of a delta time step equal to one ($\Delta t/\Delta t$),

$$-\mathbf{C}_{n\times n}\left(\frac{\Delta t}{\Delta t}\right)\mathbf{x}_{n\times 1} = \mathbf{z}_{n\times 1} \tag{43}$$

The time interval introduced in Eqs. (41) and (43) has one practical constraint,

$$\frac{\Delta t T_i^{\text{out}}}{x_i} \leq 1, \quad i = 1,2,\ldots,n \tag{44}$$

assuring the selected discrete time step does not permit more than the total stock stored in each compartment to be moved during one time step interval. Thus, the necessary constraint for an appropriate time step is established as,

$$\Delta t \leq \frac{x_i}{T_i^{\text{out}}}, \quad i = 1,2,\ldots,n \tag{45}$$

Considering the pursuit of a converging series format and with the appropriate constraints applied to Δt, first rearrange and rewrite Eq. (43) by adding and subtracting the identity matrix:

$$[-\mathbf{C}_{n\times n}\Delta t + \mathbf{I}_{n\times n} - \mathbf{I}_{n\times n}]\mathbf{x}_{n\times 1} = \mathbf{z}_{n\times 1}\Delta t \tag{46}$$

substituting (41),

$$[\mathbf{I}_{n\times n} - \mathbf{P}_{n\times n}]\mathbf{x}_{n\times 1} = \mathbf{z}_{n\times 1}\Delta t \tag{47}$$

and solve for $\boldsymbol{x}$,

$$\mathbf{x}_{n\times 1} = [\mathbf{I}_{n\times n} - \mathbf{P}_{n\times n}]^{-1}\mathbf{z}_{n\times 1}\Delta t \tag{48}$$

For convenience define $\mathbf{Q}$,

$$\mathbf{Q} \equiv [\mathbf{I} - \mathbf{P}]^{-1} \tag{49}$$

allowing (48) to be written,

$$x_{n\times 1} = \mathbf{Q}_{n\times n}\mathbf{z}_{n\times 1}\Delta t, \tag{50}$$

for all $\Delta t \le \frac{x_i}{T_i^{\text{out}}}$ per (45). $\mathbf{Q}$ represents the integral storage flow matrix [similar to $\mathbf{N}$ in Eqs. (19)–(21)] for discrete time inputs, $\mathbf{z}\Delta t$. $\boldsymbol{Q}$ accounts for all direct and indirect storage transfers as it can be alternately written:

$$\mathbf{Q} = [\mathbf{I} - \mathbf{P}]^{-1} = \mathbf{P}^0 + \mathbf{P}^1 + \mathbf{P}^2 + \mathbf{P}^3 + \cdots + \mathbf{P}^m = \sum_{m=0}^{\infty}\mathbf{P}^m \tag{51}$$

where the term $[\mathbf{I} - \mathbf{P}]^{-1}$ is expanded to the converging series $\mathbf{P}^0 + \mathbf{P}^1 + \mathbf{P}^2 + \mathbf{P}^3 + \cdots + \mathbf{P}^m$ for $m \to \infty$ if the condition $0 \le p_{ij} \le 1$ exists (for $i, j = 1, 2, \ldots, n$), which is assured if the time interval criterion of Eq. (45) is maintained. The storage-specific series (51) confers and confirms an infinite connectivity (in the limit) of indirect relationships between the storages of all system compartments. Patten's output-oriented storage environs are therefore implicit in the $\mathbf{Q}$ matrix. Each compartment's efferent connectivity first establishes a reference to the outside system through the input boundary flow $\mathbf{z}$ and then maps this boundary flow time-forward through the output-oriented environ network of all direct and indirect connections as $m \to \infty$. For continuous-time inputs $\mathbf{z}$, the integral storage matrix $\mathbf{Q}$ and the discrete time step Δt are first combined to form $\mathbf{S}$ by definition,

$$\mathbf{S}_{n\times n} \equiv \mathbf{Q}_{n\times n}\Delta t \tag{52}$$

and (50) can be written,

$$\mathbf{x}_{n\times 1} = \mathbf{S}_{n\times n}\mathbf{z}_{n\times 1} \tag{53}$$

where $\mathbf{S}$ is comprised of partial turnover times $\hat{\tau}_{ij}$ (reciprocals of partial turnover rates, $\hat{\rho}_{ij}$) mapping time-continuous inputs $\mathbf{z}$ into compartment storages, $\mathbf{x}$. Each coefficient s_{ij} represents the amount of storage generated at compartment i by a unit boundary (environmental) input to compartment j. Comparing (53) with (43) reveals,

$$\mathbf{S} = -\mathbf{C}^{-1} \tag{54}$$

Although closely related, the $\mathbf{C}$ and $\mathbf{S}$ matrices were introduced by definition separately to aid algebra, physical interpretation, and presentation. Very similar in scope to time-forward storage equation development, the afferent or time-backward steady-state storage equation development is slightly abbreviated.

2.2.2. Time-backward: $\boldsymbol{S}'$ matrix

Time-backward steady-state storage equations tracing output flows $\mathbf{y}$ backward to storages $\mathbf{x}$ are developed in the same format as the time-forward equations. By definition, the total compartment's recipient-specific turnover rate at steady-state is,

$$\rho'_i \equiv \frac{T_i^{\text{in}}}{x_i}, \quad i = 1, 2, \ldots, n \tag{55}$$

where T_i^{in} is the total steady-state throughflow into a recipient compartment i and x_i is the total steady-state storage at i. Recall, $\rho'_i = \rho_i$ at steady-state conditions. The recipient-specific partial turnover rate is defined,

$$\hat{\rho}'_{hi} \equiv \frac{f_{hi}}{x_h}, \quad h = 1, 2, \ldots, n, \; i = 1, 2, \ldots, n \tag{56}$$

where f_{hi} is intercompartmental flow to receiver h from donor i and x_h is the storage at receiver compartment h. The reciprocal of partial turnover rate $\hat{\rho}'_{hi}$ is partial turnover time $\hat{\tau}'_{hi}$ which represents compartment h's storage turnover time attributed specifically to the partitioned intercompartmental flow from compartment i directed towards compartment h. Individual partitioned turnover rates combine to equal the total compartment-specific turnover rate,

$$\rho_h = \rho'_h = \sum_{i=1}^{n}\hat{\rho}'_{hi} + \frac{z_h}{x_h}, \quad h = 1, 2, \ldots, n, \; i = 1, 2, \ldots, n \tag{57}$$

Substitute (55) and (56) into (23),

$$\rho_i x_i = \sum_{h=1}^{n}\hat{\rho}'_{hi}x_h + y_i, \quad i = 1, 2, \ldots, n \tag{58}$$

or expressed in matrix form generates

$$[x_1 \cdots x_n] \times \begin{bmatrix} \rho_1 & 0 & \cdots & 0 \\ 0 & \rho_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \rho_n \end{bmatrix} = [x_1 \cdots x_n] \times \begin{bmatrix} \hat{\rho}'_{11} & \hat{\rho}'_{12} & \cdots & \hat{\rho}'_{1n} \\ \hat{\rho}'_{21} & \hat{\rho}'_{22} & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \hat{\rho}'_{n1} & \cdots & \cdots & \hat{\rho}'_{nn} \end{bmatrix} + [y_1 \cdots y_n] \tag{59}$$

Combine similar terms to generate (60),

$$[x_1 \quad x_2 \quad \cdots \quad x_n] \times \begin{bmatrix} \left(\rho_1 - \hat{\rho}'_{11}\right) & -\hat{\rho}'_{12} & \cdots & -\hat{\rho}'_{1n} \\ -\hat{\rho}'_{21} & \left(\rho_2 - \hat{\rho}'_{22}\right) & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ -\hat{\rho}_{n1} & \cdots & \cdots & \left(\rho_n - \hat{\rho}'_{nn}\right) \end{bmatrix} = [y_1 \quad y_2 \quad \cdots \quad y_n] \tag{60}$$

The composite matrix $\mathbf{C}'$, comprised of the recipient controlled, input-oriented, partial turnover rates joined with the total turnover rates on the diagonals is defined as,

$$[\mathbf{C}'] \equiv \begin{bmatrix} -\left(\rho_1 - \widehat{\rho}'_{11}\right) & \widehat{\rho}'_{12} & \cdots & \widehat{\rho}'_{1n} \\ \widehat{\rho}'_{21} & -\left(\rho_2 - \widehat{\rho}'_{22}\right) & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \widehat{\rho}'_{n1} & \cdots & \cdots & -\left(\rho_n - \widehat{\rho}'_{nn}\right) \end{bmatrix} \tag{61}$$

Substitute $\mathbf{C}'$ into (60),

$$\mathbf{x}_{1\times n}[-\mathbf{C}']_{n\times n} = \mathbf{y}_{1\times n} \tag{62}$$

and multiply by a ratio of a delta time step equal to one ($\Delta t/\Delta t$),

$$\mathbf{x}_{1\times n}[-\mathbf{C}']_{n\times n}\left(\frac{\Delta t}{\Delta t}\right) = \mathbf{y}_{1\times n} \tag{63}$$

Pursuing a converging series format similar to (21), (31) and (51), a non-dimensional $\boldsymbol{P}'$ is defined:

$$\mathbf{P}'_{n\times n} \equiv \mathbf{I}_{n\times n} + \mathbf{C}'_{n\times n}\Delta t \tag{64}$$

where $\mathbf{I}$ is the identity matrix. The time interval constraint is

$$\frac{\Delta t T_i^{\text{in}}}{x_i} \le 1, \quad i = 1,2,\ldots,n \tag{65}$$

which assures the turnover rates ρ_i over one time step are not larger than the available stocks $\mathbf{x}_i$. The necessary constraint becomes:

$$\Delta t \le \frac{x_i}{T_i^{\text{in}}}, \quad i = 1,2,\ldots,n \tag{66}$$

Pursuing a converging series format to facilitate the decomposition of the afferent storage transfer, rearrange and rewrite Eq. (63) by adding and subtracting the identity matrix,

$$\mathbf{x}_{1\times n}[-\mathbf{C}'_{n\times n}\Delta t + \mathbf{I}_{n\times n} - \mathbf{I}_{n\times n}] = \mathbf{y}_{1\times n}\Delta t \tag{67}$$

substitute (64),

$$\mathbf{x}_{1\times n}[\mathbf{I}_{n\times n} - \mathbf{P}'_{n\times n}] = \mathbf{y}_{1\times n}\Delta t \tag{68}$$

and solve for $\mathbf{x}$,

$$\mathbf{x}_{1\times n} = \mathbf{y}_{1\times n}\Delta t[I_{n\times n} - \mathbf{P}'_{n\times n}]^{-1} \tag{69}$$

For convenience, $\mathbf{Q}'$ is defined as,

$$\mathbf{Q}' \equiv [\mathbf{I} - \mathbf{P}']^{-1} \tag{70}$$

then rewrite (69) as,

$$\mathbf{x}_{1\times n} = \mathbf{y}_{1\times n}\Delta t\mathbf{Q}'_{n\times n'} \tag{71}$$

for all $\Delta t \le (x_i/T_i^{\text{in}})$ as per (66). $\boldsymbol{Q}'$ represents the integral storage matrix [similar to $\mathbf{N}'$ in (29)–(31)] for discrete time outputs, $\boldsymbol{y}\Delta t$. $\boldsymbol{Q}'$ can alternatively be written as,

$$\mathbf{Q}' = [\mathbf{I} - \mathbf{P}']^{-1} = \mathbf{P}'^0 + \mathbf{P}'^1 + \mathbf{P}'^2 + \mathbf{P}'^3 + \cdots + \mathbf{P}'^m = \sum_{m=0}^{\infty} \mathbf{P}'^m \tag{72}$$

where the term $[\mathbf{I} - \mathbf{P}']^{-1}$ is expanded to the convergent series $\mathbf{P}'^0 + \mathbf{P}'^1 + \mathbf{P}'^2 + \mathbf{P}'^3 + \cdots + \mathbf{P}'^m$ for $m \to \infty$ if the condition $0 \le p'_{ij} \le 1$ exists (for $i, j = 1, 2, \ldots, n$), which is assured if the time interval criterion as per Eq. (66) is maintained. The input-oriented storage environs are implicit in the $\boldsymbol{Q}'$ matrix. Each compartment's afferent connectivity, in a multi-compartment system, is first referenced to the outside system through the output boundary flow $\boldsymbol{y}$ and then subsequently mapped time-backwards from this boundary flow through its input-environ network of compartment storages through all direct and indirect connections as $m \to \infty$. For continuous-time outputs $\boldsymbol{y}$, the integral storage matrix $\boldsymbol{Q}'$ and the discrete time step Δt are combined to form $\boldsymbol{S}'$ by definition,

$$\mathbf{S}'_{n\times n} \equiv \mathbf{Q}'_{n\times n}\Delta t \tag{73}$$

such that (71) can be written as,

$$\mathbf{x}_{1\times n} = \mathbf{y}_{1\times n}\mathbf{S}'_{n\times n} \tag{74}$$

$\mathbf{S}'$ maps the time-continuous outputs $\mathbf{y}$ from compartment storages $\mathbf{x}$. Comparing (74) with (62) reveals,

$$\mathbf{S}' = -\mathbf{C}'^{-1} \tag{75}$$

$\mathbf{S}'$ is comprised of integral turnover times, $\widehat{\tau}_{hi}$, mapping time-continuous outputs $\mathbf{y}$ from compartment storages, $\mathbf{x}$. Each coefficient s'_{ij} represents the amount of storage that needs to be generated at compartment j for a unit boundary (environmental) output from compartment i.

2.3. Utility analysis: *U* matrix

Utility analysis elicits relationships among n-compartment network systems. From the dimensionless flow utilities defined as:

$$\mathbf{D} = d_{ij} \equiv \frac{\left(f_{ij} - f_{ji}\right)}{T_i}, \quad j = 1,2,\ldots,n; \; i = 1,2,\ldots,n \tag{76}$$

the dimensionless integral utility intensity matrix is computed:

$$\mathbf{U} = [\mathbf{I} - \mathbf{D}]^{-1} = \mathbf{D}^0 + \mathbf{D}^1 + \mathbf{D}^2 + \mathbf{D}^3 + \cdots + \mathbf{D}^m = \sum_{m=0}^{\infty} \mathbf{G}^m \tag{77}$$

Networks whose largest eigenvalue of $\mathbf{D}$ are not less than one [convergence does not exist using (77)] are excluded from utility analysis. For further details on utility analysis, and NEA in general, we refer the reader to references (Fath and Patten, 1999; Fath and Borrett, 2006; Patten, in prep.).

2.4. Control analysis: *CR* and *CD* matrices

Control or dominance analysis, originated by Patten (1978) and advanced by others (Patten and Auble, 1981; Patten, 1982; Fath, 2004) is shown here from Schramski (2006) and Schramski et al. (2006, 2007) where the fractional transfer coefficients η_{ij} and η_{ji} are by definition:

$$\eta_{ij} \equiv \left[\frac{n_{ij}}{T_i^{\text{out}}}\right], \quad i,j = 1,2,\ldots,n \tag{78}$$

$$\eta_{ji} \equiv \left[\frac{n_{ij}}{T_i^{\text{out}}}\right], \quad i,j = 1,2,\ldots,n \tag{79}$$

Note, on the left-hand sides, the use of the Greek letter eta η for the fractional transfer coefficients, specifically differentiating from the Arabic n used throughout the text for the integral flow matrix values. Pair-wise component comparisons are enabled by a dimensionless *control ratio* (Patten, 1978):

$$\mathbf{CR} = \mathrm{cr}_{ij} \equiv \frac{\eta_{ij} - \eta_{ji}}{\max\left(\eta_{ij}, \eta_{ji}\right)}, \quad i,j = 1,2,\ldots,n, \ 0 \le \left|\mathrm{cr}_{ij}\right| \le 1 \qquad (80)$$

and system-based comparisons of the fractional transfer values are made with the *control difference* (Schramski et al., 2006):

$$\mathbf{CD} = \mathrm{cd}_{ij} \equiv \eta_{ij} - \eta_{ji}, \quad i,j = 1,2,\ldots,n, \ 0 \le \left|\mathrm{cd}_{ij}\right| < \infty \qquad (81)$$

These metrics compare the integral flows from i to j to that from j to i over all paths of all path-lengths. Compartment j controls or dominates i if its output environ effect on i from j (j looking forward through the network specifically at i) is larger than its corresponding input-environ effect on j from i (j looking backward through the network specifically at i).

3. Structural analysis—adjacency matrix

A simple binary matrix of ones and zeros facilitates a discussion of a network model's pathways (structure) and the corresponding concept of pathway proliferation. The appropriately titled adjacency matrix from mathematical graph theory, $\mathbf{A} = (a_{ij})$, sometimes called an interconnection matrix (Šiljak, 1991), represents a system's direct compartment connectivity. Values of $a_{ij} = 1$ and $a_{ij} = 0$ signify flow and no flow connections from compartment j to i. Therefore, the flow matrix $\mathbf{F} = (f_{ij})$ is algebraically homomorphic to the $\mathbf{A}$ matrix where an infinite number of $\mathbf{F}$'s can be mapped into the same $\mathbf{A}$. The adjacency matrix raised to the mth power, $\mathbf{A}^m$ *or* $(a_{ij})^m$ (matrix multiplication not scalar powers), enumerates quantities of pathways of length m directed from each j to each i in the system. Specifically, the whole number in an (i, j) interstitial location of the matrix $(a_{ij})^m$ is the number of indirect pathways between compartments j and i of path length m where the (i, j) entry of $(a_{ij})^m$ is denoted $a_{ij}^{(m)}$ by standard notation. In general, values of $a_{ij}^{(m)}$ increase without bound as $m \to \infty$, signifying that the quantity of indirect pathways between j and i increase without bound as path length m increases. Pathway proliferation analysis (e.g., Patten, 1985) systematically evaluates increasing powers of the adjacency matrix for trends with indirect connectivity between various compartments in a multi-compartment system. For example, Borrett and Patten (2003) and Borrett et al. (2007) relate proliferation tendencies to the number of strongly connected compartments and the dominant eigenvalue of the matrix.

4. EcoNet—ecological network analysis (ENA) software

EcoNet simplifies model building, simulation, and analysis efforts. The software's easy interface encourages first-time modelers to access a powerful modeling tool while minimizing model-building efforts for experienced users, thus closing the gap between model development and results for all users. EcoNet's flow currency usually is energy, biomass, or a specific element such as C, N, or P. Storage compartments represent anything from accumulated organic matter to a group of species where any process represented as a stock-flow diagram, related to biology, ecology, economics, etc. can be implemented in EcoNet within minutes. EcoNet performs deterministic or stochastic dynamic simulation from a given initial condition, and then performs ecological network analysis after the system reaches steady-state. The regular simulation results are displayed on the first output page generated from the "Run Model" activation at the website. Extended simulation and analysis results are provided by clicking the "Show Extended Results" option at the top of the regular simulation results page. While EcoNet results can be viewed online, simulation results are automatically exported into both a CSV file and an M-file. A CSV file is useful if the user wishes to do further work using spreadsheet software such as OpenOffice or MS Excel. Users can also work in Octave or Matlab using the provided M-file (e.g., Tollner et al., 2009). By simply clicking on the figures, users can download publication quality vector-based versions of the figures which are in EPS format.

4.1. EcoNet—model input

Model initiation is designed to be intuitive. The software launch requires initial compartment storage quantities x_i, input boundary flows z_i, and flow-rate-control coefficients for intercompartmental and output boundary flows. Determine the flow control type (donor, donor-recipient, etc.) for the flow-rate-control coefficients [e.g., Eq. (33)] and simply input the model parameters per the software's guidance on the main screen.

4.2. EcoNet—model parameter input and model execution

After the model input data is entered, choose a numerical solution method, adjust the *Sensitivity* or *Total Time* parameters if necessary, and click "Run Model". EcoNet generates a multiple differential equation system (number of model compartments determines number of equations) using Eq. (2). In most cases the default algorithm (Runge–Kutta–Fehlberg) and parameters (*Sensitivity* at 0.001, *Total Time* at 100 steps) will work to sufficiently model the system activity, and no adjustments are necessary. Runge–Kutta–Fehlberg is an adaptive scheme that continuously optimizes its speed and accuracy to the complexity of the solution. Any problems with the solution are usually remedied by adjusting the *Sensitivity* parameter which correlates the amount of error allowed between the actual and numerical solutions. *Total Time* (not to be confused with the actual time it takes EcoNet to run the simulation) is basically the maximum time or simulation length of the model duration with dimensional units of time. The user defined model input data and parameters and one of the four user defined numerical simulation methodologies are used to solve and plot the dynamically evolving system which starts from the initial storage values. Given sufficient run time (*Total Time*), most models, but not all, will eventually settle into a steady-state system of unchanging final compartment storage quantities, x_i.

4.3. EcoNet results—network diagram pictorial

EcoNet's first figure displays the model's network diagram which provides visual information lacking in the thus far text-based EcoNet format. Existing compartment modeling software in general uses a graphical model-building interface. Users drag and drop geometrical shapes representing compartments and subsequently define arrows connecting these compartments providing the requisite visual information for system connectivity. However, with slightly larger systems, a finished model often has too many flow lines crossing each other, creating a less helpful representation. Thus the model is hard to build and the final appearance is hindered. Using Graphviz (Ellson et al., 2003), EcoNet automatically and purposely provides system insight into both system structure and functionality by locating important highly connected storages in the center, while keeping less connected storages closer to the edges. Flow lines are short, with little curvature, and minimal intersections. Tightly coupled compartments, in large systems, are located close to each other. When possible, locations of compartments reflect their trophic level. EcoNet diagrams are designed to look as clean as possible and work with large models with over 50 compartments and 100 flows.

4.4. EcoNet results—graph of compartment storage variation

EcoNet's second figure is a time-course plot (x-axis is $0.0 \leq t \leq$ Total Time) of initial to final compartment storages. EcoNet provides access to the actual time-course data via an html-link "Data for time-course figure" located underneath this graph.

Advanced users are cautioned not to confuse a stochastic solution with a deterministic solution driven by a noisy input, or a deterministic solution perturbed randomly at each iteration step. Although these practices will generate random behaving solutions, the noise-term associated with these solutions is wrong, which negates the very advantage of using a stochastic solution method in the first place. This is not a trivial fact, and we refer the interested user to further reading (Gillespie, 2000; Gardiner, 1985). Simply, a stochastic process representing a stock-flow model should be compatible with the so-called *master equation* (Gillespie, 1992). This is not an easy condition to satisfy, and true stochastic solvers are complex and hard to implement. This is the main reason why very few software programs feature stochastic methods. As they are not widely available, few users are aware of their power. For example, a single stochastic solution will reveal the inherent variations in the stock values, eliminating the need for many repeated runs for sensitivity analysis. It seems that stochastic solutions always look like the noisy versions of their deterministic versions. This is not true in general; cases exist where only a stochastic method will provide an accurate representation of the modeled system. For example, if the flowing matter in the system exists in scarce discrete quantities, or if the system is capable of multiple steady-states, deterministic and stochastic methods may differ significantly.

4.5. EcoNet results—structural, functional, and storage analysis

Assuming a sufficiently steady-state solution is achieved, the software returns the Adjacency matrix $\mathbf{A}$, the intercompartmental Flow matrix $\mathbf{F}$, boundary input flows z_i, final storages x_i, and final output flows, y_i. Thus, an intercompartmental model with both structure and function is established.

Where throughflow is a means to quantify compartment or system activity, EcoNet's throughflow analysis is initiated by using Eqs. (3), (4), and (6) or (7), to calculate the compartmental input T_i^{in} and output T_i^{out} throughflows and the Total System Throughflow TST. Equations (14) and (24) are used to calculate the normalized efferent g_{ij} (donor) and afferent g'_{hi} (recipient) throughflow intensity matrices. These values represent the fraction of total compartment throughflows donated or received from respective compartments. EcoNet uses Eqs. (19) and (29) to determine the efferent $\mathbf{N}_{n\times n}$ and afferent $\mathbf{N}'_{n\times n}$ integral flow matrices. The integral flow matrix $\mathbf{N}_{n\times n}$ relates the system-level boundary input vector z_i over all direct and indirect pathways to the compartmental throughflow vector $\mathbf{T}^{\text{out}}_{n\times 1}$. The integral flow matrix $\mathbf{N}'_{n\times n}$ relates the system-level boundary output vector y_i over all direct and indirect pathways back to the compartmental throughflow vector $\mathbf{T}^{\text{in}}_{1\times n}$.

Compartment storage is another method to gauge or quantify compartment and system specific activity. EcoNet's storage analysis is initiated by calculating compartment turnover time using the reciprocal of each compartment's partial and total turnover rates from Eqs. (32), (33) (55), and (56). Eqs. (40) and (61) are used to organize the input and output turnover rate matrices $\boldsymbol{C}$ and $\mathbf{C}'$. Eqs. (54) and (75) are used to determine the corresponding input and output storage matrices $\boldsymbol{S}$ and $\mathbf{S}'$.

4.6. EcoNet results—utility and control analysis

Network environ utility and control analysis elicit compartment relationships across all paths of all lengths in multi-compartment systems. The dimensionless flow utility matrix $\mathbf{D}$ and corresponding integral intensity matrix $\mathbf{U}$ are calculated with Eqs. (76) and (77). The dimensionless pair-wise control ratio $\mathbf{CR}$ and system-based control difference $\mathbf{CD}$ are calculated with Eqs. (80) and (81).

4.7. EcoNet results— accessible, emergent ecological network analysis

EcoNet is an online software package. As such, new features and updates are continuously implemented as research evolves and is published. EcoNet currently calculates Link Density (number of intercompartmental links per number of compartments), Connectance (ratio of the number of actual intercompartmental links to the number of possible intercompartmental links), Total System Throughflow [Eq. (10)], Finn's Cycling Index (Finn, 1976; Kazanci et al., 2009), Indirect Effects Index (Higashi and Patten, 1989), Ascendency (Ulanowicz, 1986; Patrício et al., 2004; Ulanowicz et al., 2006), Aggradation Index (Ulanowicz et al., 2006), Synergism Index (Fath and Borrett, 2006; Fath and Patten, 1999), Mutualism Index (Fath and Borrett, 2006; Fath and Patten, 1999), Homogenization Index (Fath and Patten, 1999), and Eco-exergy (Jørgensen, 2006; Ulanowicz et al., 2006; Jørgensen and Nielsen, 2007).

5. Discussion

This research combines the next generation of EcoNet's rapidly expanding web-based presence with the user requested clarity of the underlying model's foundational equations. EcoNet, Network Environ Analysis, Ecological Network Analysis, and their respective models are active areas of research where, with increasing use, inquiries arise almost daily with regard to EcoNet's underlying mathematics. Where Fath (2004) notes that the computational portion of network analysis is not daunting, we therefore address and continuously improve both the user interface and the availability and clarity of the underlying mathematical construction. The user improvements and respective equation developments herein facilitate the presentation of Ecological Network Analysis to a wider audience. EcoNet was accessed by over 1200 unique users in calendar year 2008 from over 50 countries. With these ongoing improvements, EcoNet's use is increasing again in 2009 where environmental modeling's virtual databases and web-based software in general are improving and increasing user availability and software designer flexibility (e.g., Frehner and Brändli, 2006; Bianconi et al., 2004; Rao et al., 2007; Dawson et al., 2007, 2010).

Although developed in parts in many publications, these equation derivations are subtly different than recent trends as they reach back to the original development initiated in Barber et al. (1979). In particular, we focus first on the law of conservation, then substitute the definition of throughflow, and then algebraically derive each model parameter or representation from these original flow representations recognizing that Ecological Network Analysis is fundamentally a conservation law analysis. The input or output environ orientating capability of Network Environ Analysis is then a fundamental and readily visible construct of the in- and out-oriented nature of the conservation and throughflow equation's terms.

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