AC 2007-1345: AN EVOLVING COURSE IN ECOLOGICAL THERMODYNAMICS

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An Evolving Course in Ecological Thermodynamics

Ernest W. Tollner and Caner Kazanci

Abstract

The ecological thermodynamics course at the University of Georgia has served as a platform for developing a novel Lagrangian type ecological thermodynamics approach that mimics the statistical thermodynamics approach in that it attempts to focus on system state before and after a process. The Lagrangian approach compliments the classical process-based thermodynamic approach that focuses on the thermo-mechanical processes involved in changing a system state. The conduct of an entropy analyses has proven to be beneficial in that it provides an independent look at the energy budget. The seminar environment has proven useful for faculty and students with a non-engineering background to grasp the fundamentals of thermodynamics. The experience continues to bring to light pedagogical approaches that can be useful to making one of the most dreaded engineering science courses more palatable to engineering students.

Introduction

Can thermodynamic principles enable a qualitative basis for ecological engineering design? New insights into interdisciplinary engineering endeavors, from classical modeling to nano – macroscale extrapolation and critical evaluation, weigh heavily on the pervasive nature of thermodynamics in the physical world. Concepts being developed in the Systems Ecology program at the University of Georgia provide the basis for interdisciplinary thermodynamics research in a seminar format, with periodic oral and written reports to educate classmates on student findings. An important component of the course is new approaches for bridging the gap between an increasingly popular technique known as network environ analysis and current works in ecological thermodynamics. The seminar tackles concepts in a typical engineering thermodynamics course that are relevant to science in general. We then explore some concepts of statistical thermodynamics that were successful in predicting thermodynamics of gases and solids based on molecular considerations.

The first offering of the course left us with the impression that classical approaches to applying entropy were less than satisfying, particularly when large temporal and geographic scales were involved. Statistical mechanics can be used to predict thermodynamic properties when homogeneity and near equilibrium conditions can be reasonably assumed. Living systems with all their complexities add layers of complications. The purpose of this paper is to explore an analogue of statistical thermodynamics on an ecological scale and see how it compliments classical thermodynamic analyses.

The presentation will explore success and other directions taken in this course based on a fall 2006 offering. The pedagogical approach has been a loosely structured seminar that seems appropriate. The syllabus is summarized as follows:

- Gain a qualitative understanding of terminology, the first law, the second law from an introductory text (We used Whalley, 1992). We also focused on worked examples of first and second law analyses found in Cengel and Boles (2002).

- Spend two days per week covering fundamentals in ecological thermodynamics (Jorgenson and Svirezhev, 2004) and spend one day per week analyzing papers of Ichiru Aoki and other leaders in the field.

- Students tackled a project based on the papers for a detailed energetics analyses as a final project

The course considered the laws of thermodynamics in the classical sense and investigated some models showing how these laws describe solids and gases at the microscopic level in the context of isolated, closed and open systems. We addressed the difficulties of extrapolating from nanoscale to macro scale, critically evaluating the implications of the scale change as related to the laws. We evaluated the impact of departing from near-equilibrium conditions to far-from-equilibrium conditions.

The seminar set forth the following broad objectives:

*Appreciate the pervasive nature of the laws of thermodynamics and how these first principles may serve as a basis for interdisciplinary science/engineering research.

*Appreciate the potentials and pitfalls of 1) scale-ups and 2) departures from equilibrium on reasonable application of the laws of thermodynamics.

Briefly, we concluded that in order to build a rigorous basis for physically based design, ecological or otherwise, one must begin with energetics. The system must be clearly defined, thermodynamic coordinates must be identified and an effective equation of state must be developed. Thermodynamic coordinates may include temperature, energy, constituents and possibly ecological orientors. One may then analyze many systems to determine the relative robustness of the coordinate set. As trends begin to emerge, ecological engineering will be on its way to taking its place with other engineering disciplines.

The literature surveyed suggests that yes; we can apply thermodynamic principles to develop a quantitative basis for design. The seminar likewise revealed some insights for so doing. This energetics seminar has served well to identify many of the required bases for commencing this effort. We must now set our sights towards this task.

An underlying sense pervaded that basing our definition of thermodynamic principles on molecular and atomic behavior was insufficient to describe ecological problems. Additional approaches were required to enable scaling from the molecular to the ecological temporal and spatial levels. The fundamental definition of entropy is based on a statistical distribution of molecular and atomic states. Once the distributions become multimodal, scale-up becomes problematic without some additional tools. The purpose of this presentation is to introduce an inquiry that may lead to new approaches for analyzing thermodynamics of ecosystems. The approach will be oriented around network environ analyses (Patten, 1978; Gattie et al., 2005) and will be augmented by an alternative analyses based on a Lagrangian approach. The thrust of this paper is not to focus on thermodynamic fundamentals as was done in Tollner and Kazanci (2006) but instead to focus on broader issues related to how the ecological Lagrangian approach compliments a conventional macroscopic thermodynamic approach.

Lagrangian Analyses of two Ecological Systems

Programming SIMON/ARENA to track individual elements is a relatively cumbersome task because of the minute control requirements. An advanced modeling and differential equation solution package known as 'ECONET' (see Kazanci, 2006) has been configured to solve systems of deterministic or stochastic differential equations with particle tracking (Kazanci and Tollner, 2006). ECONET is similar to STELLA in that it provides solutions to a series of first order continuous ODEs arising from typical control volume analyses. Rather than the detailed process programming required by SIMON/ARENA, ECONET uses a chemical mass action approach for managing the movement of energy or mass packets (or quanta) from one node to the next.

The important ECONET enhancement now available is the capability of solving stochastic ODEs based on Gillespie's stochastic algorithm (Gillespie, 1977). A particle-tracking feature now under development enables Lagrangian-type particle tracking. We are applying the ECONET Lagrangian particle tracking approach to an ecological thermodynamic analysis of two well-publicized data sets: Cone Springs (Ulanowicz, 2000) and Oyster reef (Dame and Patten, 1981).

The Cone Springs model is shown schematically in Figure 1. The ECONET model was run two different times with two different packet sizes. An indication that a robust steady state values of stocks was reached was that the total number of packets in the system was about 6900 in both runs with similar distributions among the nodes. The nodes in the analyses included plants, bacteria, detritivors, carnivors and detritus. Results for one run are shown in Figures 1-4. Figure 2 shows the path from a starting condition to steady state. Steady state was reached in approximately 0.5 time units. The number of iterations over two time units was about 137,000. Particles passing through the system numbered about 34,000. Histograms of packet numbers vs. nodal contacts are shown in Figure 3. A composite histogram of packet numbers vs. nodal contacts is shown in semilog form in Figure 4. The results for individual nodes takes on the shape of the Maxwell-Boltzmann distribution and the linear tail in Figure 4 follows from the log transform. The detritus node was dominating in this model.
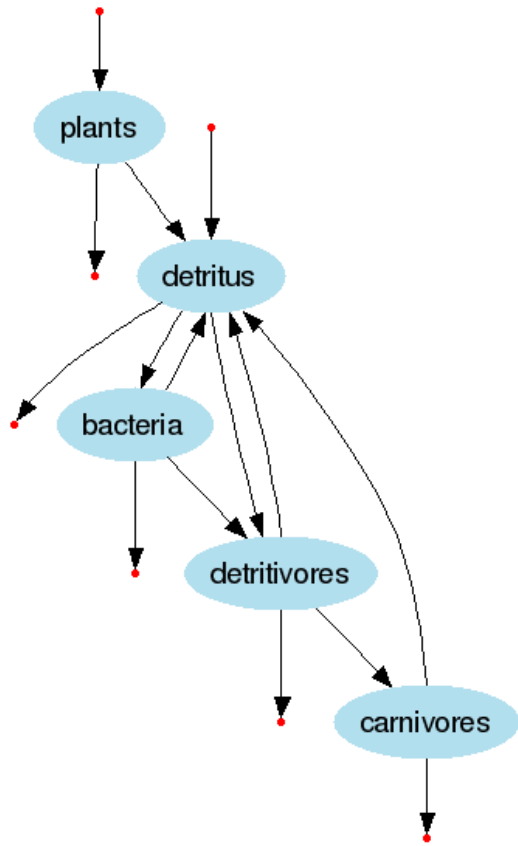
Figure 1. Schematic of the Cone Springs model as rendered by ECONET.
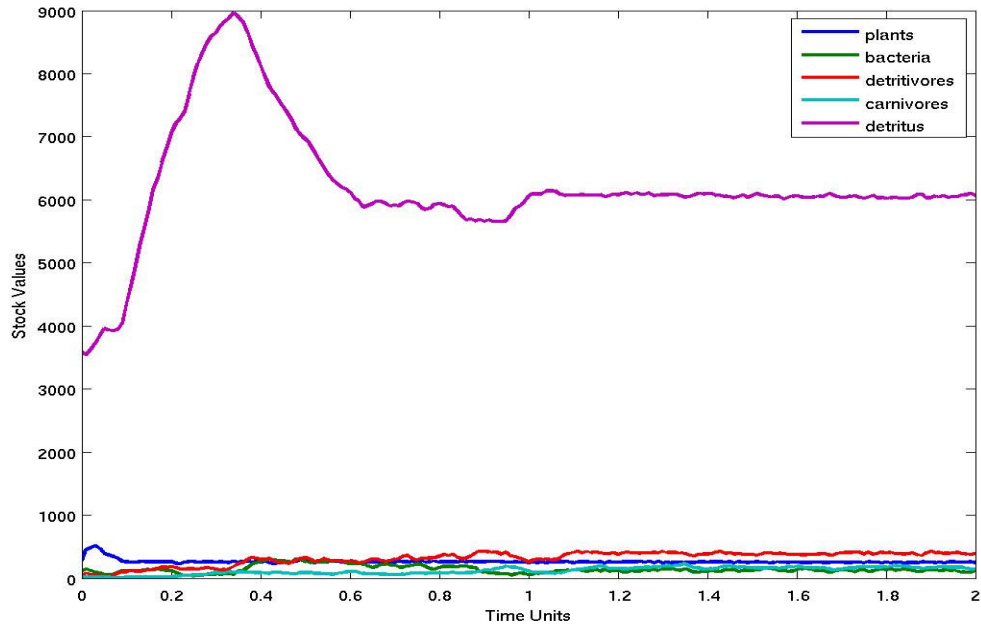
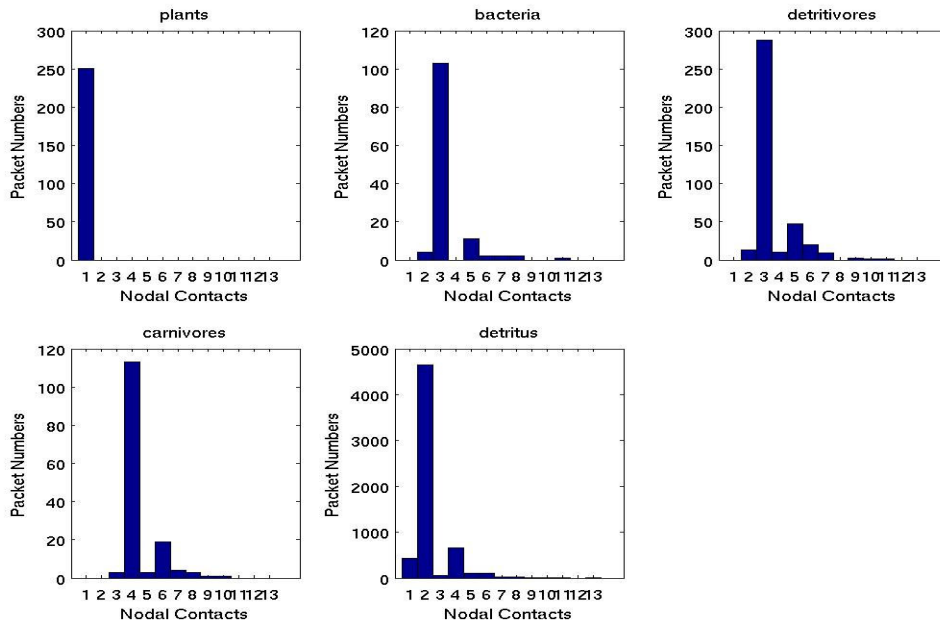Figure 2. Stock values vs. time units in a Cone Springs ECONET model run.

Figure 3. Final plot matrix of packet numbers vs. nodal contacts by node for the Cone Springs model run shown in Figure 2.
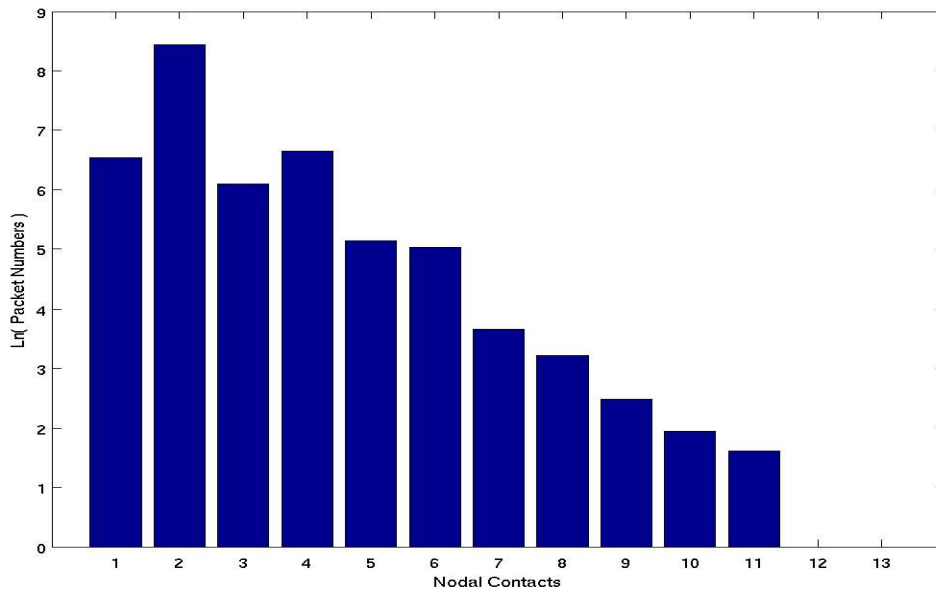
Figure 4. Cumulative plot of the natural logarithm of packet numbers versus nodal contacts for the Cone Spring model run of Figure 2.

Table 1. Summary of Nodal Inputs and Actions for the Cone Springs model run of Figure 2.

Node	SE_{inform}	SE_{Boltz}	S_{Macro}
Bacteria	1.04	23.30	11.18
Carnivores	1.26	27.57	0.69
Detritivors	1.42	33.45	6.19
Detritus	1.27	59.10	10.61
Plants	0.00	0.00	6.84
Total System	**1.68**	**55.39**	
Nodal Sum	**4.99**	**143.42**	**35.51**

Note: The energy units are kcal/m^2 – yr
An arbitrary value of 1.0 is assigned to the Boltzmann constant.

The Oyster model is shown schematically in Figure 5. The ECONET model was run two different times with two different packet sizes. An indication that a robust steady state values of stocks was reached was that the total number of packets in the system was about 40,000 in both runs with similar distributions among the nodes. The nodes in the analyses included filter feeders, deep detritus, microbiota, meofauna, deep feeders and predators. Results for one run are shown in Figures 6-8. Figure 6 shows the path from a starting condition to steady state. Steady state was reached in approximately 1000 time units. The number of iterations over two time units was about 3.2 million. Particles

passing through the system numbered just over 1 million. Histograms of packet numbers vs. nodal contacts are shown in Figure 7. A composite histogram of packet numbers vs. nodal contacts is shown in semilog form in Figure 14. The results for individual nodes takes on the shape of the Maxwell-Boltzmann distribution and the linear tail in Figure 14 follows from the log transform. The filter feeders node followed by the deep detritus node was dominating in this model.
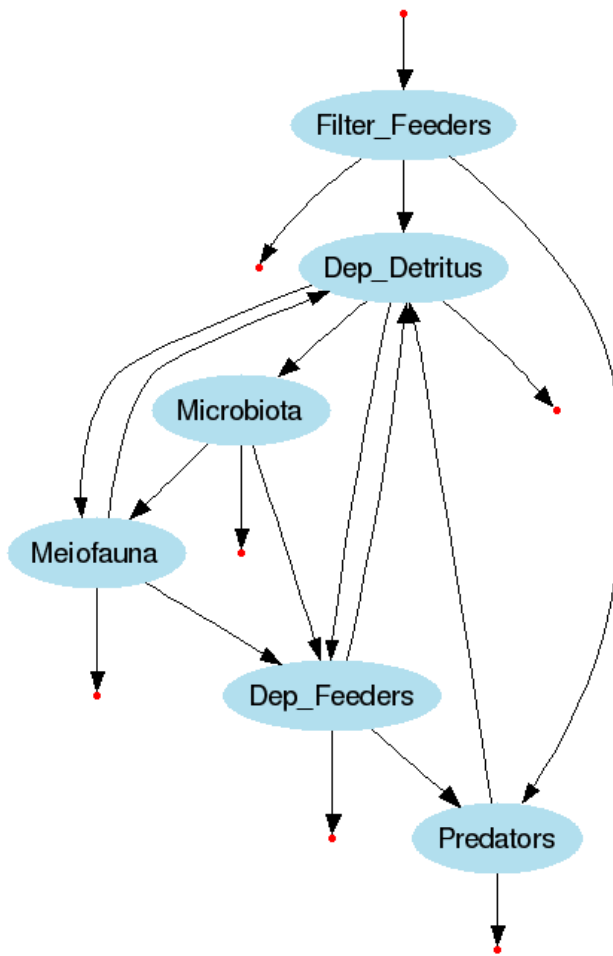

Figure 5. Schematic of the Oyster reef model as rendered by ECONET.
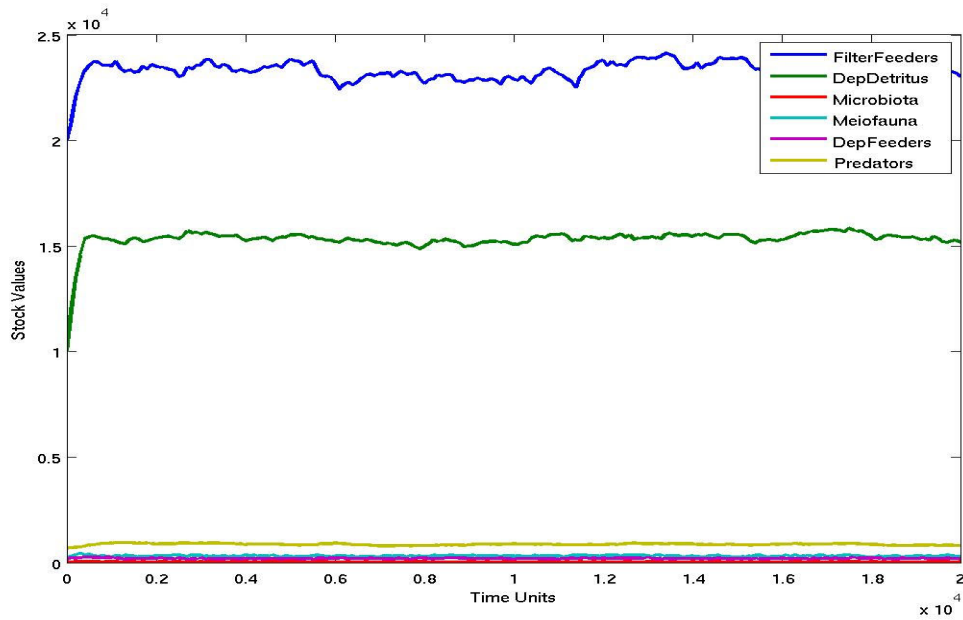
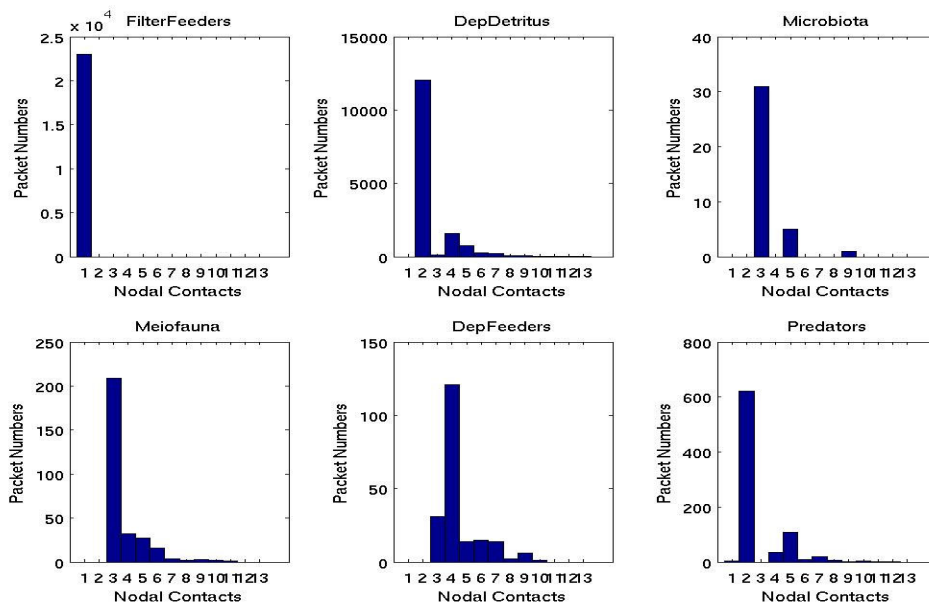Figure 6. Stock values vs. time units in an Oyster reef model ECONET run.

Figure 7. Final plot matrix of packet numbers vs. nodal contacts by node for the Oyster model run in Figure 5.
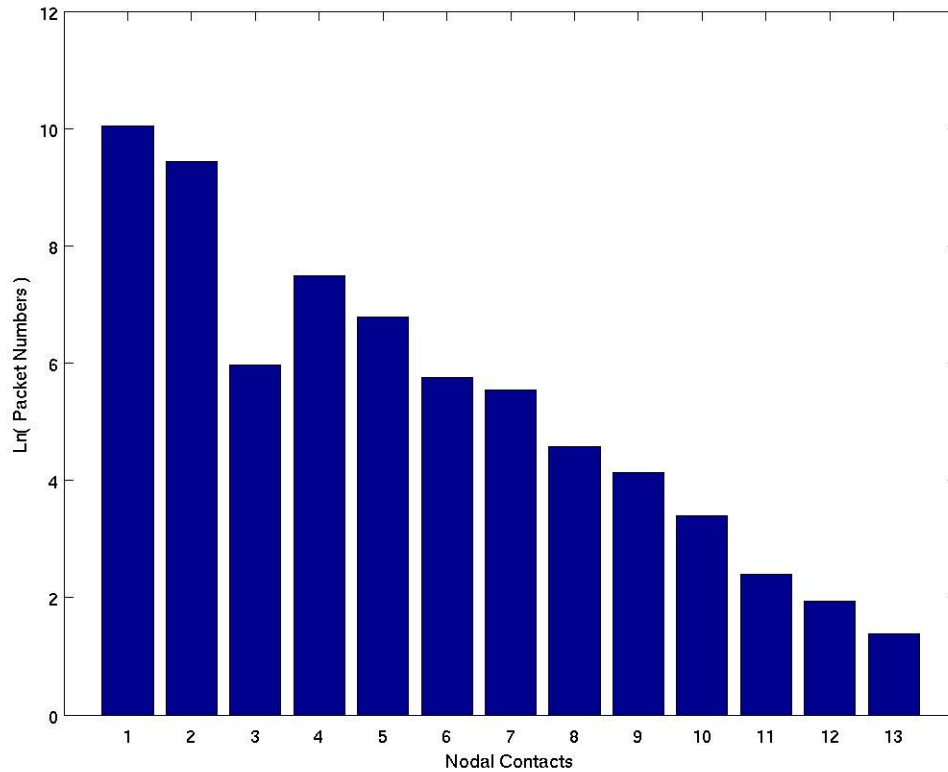
Figure 8. Cumulative plot of the natural logarithm of packet numbers versus nodal contacts for the Oyster reef model run of Figure 5.

Table 2. Summary of Nodal Inputs and Actions for the Oyster model run of Figure 12.

Node	Shannon Entropy	Boltzmann Entropy	Macroscopic Entropy
FilterFeeder	0.00	0.00	31.34
Dep. Detritus	1.15	80.00	7.69
Microbiota	1.36	11.58	7.18
Meofauna	1.57	27.16	4.46
Dep. Feeders	1.94	29.15	0.54
Preditors	1.31	39.70	0.49
Total System	**1.53**	**91.05**	
Nodal Sum	**7.34**	**187.60**	**51.7**

Note: The energy units are converted from kcal/m^2 – day to kcal/m^2 – yr
An arbitrary value of 1.0 is assigned to the Boltzmann constant.

The Maxwell-Boltzmann distribution shape is discernable in the Cone Springs and Oyster models. Each model tends to be dominated by one or two nodes. It is tempting to simply add the entropy from the respective nodes; however, the more correct way appears be to accumulate the packets numbers contacting the respective node numbers and recomputed the entropy, since the logarithm is not a linear function. These results are shown in Tables 2 and 3 along with the macroscopic entropy for each node. It is interesting to note that the analysis thus far treats every node as equal in terms of effect on the energy packet. It is conceivable that one could bring to bear an appropriate Maxwell-Boltzmann type of biochemical entropy to packets leaving each node in an additional post-processing step. This may enable an addition of biochemical entropy to ecological entropy in a way that goes beyond a simple addition of the type used by Jorgensen and Svirezhev (2004) when they added biochemical and information entropy.

A summary of selected entropy ratios for all three models evaluated is shown in Table 4. The Boltzmann entropy computed using total nodal contacts in the system versus the Boltzmann entropy summed for each node (B.lumped/B.nodal) was consistent over all models. The related ratios involving Shannon entropy (Shan. lumped/Shan. Nodal) was not as consistent. The essential nonlinearity of the entropy definition is obvious in that these ratios are far from unity, as one would expect from a linear process. This raises a doubt that the sum of the entropy in a system is simply the sum of nodal entropies.

Table 3. Comparison of Shannon, Boltzmann and macroscopic entropy ratios on the indicated models.

Model	Shan. lump. / Shan. nodal	B.lump/ B. nodal	Shan. lump/ macro	B. lump/ macro	Shan. nodal/ macro	B. nodal/ macro
Tollner & Kazanci 2006	0.60	0.43	10.99	356.47	18.32	834.87
Cone Springs	0.34	0.39	0.05	1.56	0.14	4.04
Oyster	0.21	0.49	0.03	1.76	0.14	3.63

The respective comparisons of lumped/macro entropies provided consistent results in the ecological models. The Cone Springs and Oyster models had some similarity in that they were dominated by one or two nodes. There is no compelling reason to choose the Shannon information entropy over the Boltzmann entropy based on the lumped entropy/macroscopic entropy ratios. The same may be said for the nodal sum to macroscopic entropy ratios with the ecological systems. The arbitrary system shown in Table 3 represents an analyses of the system shown in Tollner and Kazanci (2006). It varied greatly, which is not surprising given the arbitrary energy units. Another contributing factor to the difference may also have been that the arbitrary system was not dominated by a single node, as were the other ecological models.

Is Ecological Thermodynamics worthwhile?

The introduction of living entities in a system complicates the estimation of entropy from a microscopic sense. The macroscopic balance is still regarded as valid, with the entropy generation term being the impacted parameter. Aoki (2001) gives an

excellent summary of efforts to compute macroscopic entropy balances in ecological systems. The above statements imply that organisms are on a trajectory leading to death.

Can we use an expanded definition of entropy to discern how an ecosystem will organize itself? With nonliving systems, the system goal functions (e.g., open systems -> minimum entropy production; closed systems -> maximum entropy) are now well understood. When life is introduced, the nature of the goal function is a subject of study (see Fath et al 2004). They tested several hypotheses involving thermodynamic description of the orientation or natural tendency that ecosystems follow during succession. Specifically, five thermodynamic orientors were tested: minimize specific entropy production, maximize dissipation and maximize exergy storage (includes biomass and information), maximize energy through flow, and maximize retention time. These thermodynamic orientors are known to be present to some degree during succession, and here we present a refinement by observing them during different stages of succession. They view ecosystem succession as a series of four growth and development stages: boundary, structural, network, and informational. They demonstrate how each of these ecological thermodynamic orientors behaves during the different growth and development stages, and show that while all apply during some stages only maximizing energy through flow and maximizing exergy storage are applicable during all four stages. It was concluded that the movement away from thermodynamic equilibrium, and the subsequent increase in organization during ecosystem growth and development, is a result of system components and configurations that maximize the flux of useful energy and the amount of stored exergy.

One must identify the nature of the system. Biological systems are generally analyzed as open systems. The first law must be satisfied in the Eulerian or Lagrangian scheme. From a Eulerian vs. statistical thermodynamic view:

- The ability to bring a construct called energy to bear in mechanical processes, electrical processes, thermal processes, chemical processes and to identify reversible work modes in each context was a crowning achievement of the late 19th century.
- A seemingly unbounded supply of high quality energy or exergy seems to be the prime driver of all that we know.
- One must account for convected heat and free energy in constituents with open systems.
- Eulerian energy balances have been very insightful across numerous science and engineering fields.

- Entropy is based on process in the macroscopic realm.
- Statistical thermodynamics provides a complementary look by introducing a characterization of state before and after a process.
- The definition of entropy is not universally accepted in a far-from-equilibrium state.
- The entropy concept was found to give consistent results with the second law in several life processes, even though life is considered by most to be far-from equilibrium.

- The second law was observed to hold in the presence of life and organization. The key was a supply of higher quality energy (or exergy; negentropy).
- Open systems must account for standard entropy in mass flows

- The integration of statistical and macroscopic thermodynamic concepts has led to a much more comprehensive understanding of matter.
- Thermodynamic temperature and pressure and equivalence to mechanically measurable temperature and pressure is a strong link between theory and practice.
- Relating other properties such as conductivity and viscosity to statistical thermodynamics further solidifies the link.
- Linking statistical and macroscopic concepts are essential.
- Statistical thermodynamics focuses on the states before and after while conventional macroscopic thermodynamics focuses on the process that is responsible for the state change.
- We wanted to get into EMERGY analyses but were unable to do so due to time constraints.

It is felt that one can link classical thermodynamics and ecological scale thermodynamics by probabilistic approaches based on Lagrangian interpretations of network environ analyses. As a step in this direction, one could consider the exergy of each input, perform the Lagrangian analyses for many pulse events and then treat each energy history as a separate energy state. One could allow the quality of the incoming energy to vary. Thermodynamic properties could be computed for each node using the weighting based on numbers of packets at particular states, A model such as Arena (see Kelton et al 2004), which is a discrete model enabling one to track attributes of individual packets, would aid in tracking the state of more complex systems. The ECONET model of Kazanci (2006) will further aid in the analyses.

Can we gain insight into how one may relate these findings to a definition of ecological entropy? These results suggest that, yes we can.

The approach needs evaluation on many other systems.

What was learned pedagogically?

It became striking to me as this course developed that most of us never consider the entropy related to sunlight. Our energy is largely come from the sun. Our introductory courses in thermodynamics for example never bring us to the point of computing the entropy of radiation-received energy. We never consider how much solar energy had to be received to result in the creation of a gallon of crude oil. I believe we need to revisit the syllabus of the basic course in thermodynamics, leaving in place the first law analyses but focusing more on the energetics of solar radiation.

Student projects suggested that they liked the energy analyses. It appeared that one benefit of the 2nd law analyses was to serve as a cross check on the energy analyses.

Failing to include a component of the energy/entropy may cause the entropy balance to be negative. Since by the 2nd law this is impossible, one looks harder at the various components of the energy balance. We believe that the entropy can be a necessary but not sufficient check on the energy balance.

We need to focus on classroom designs that foster discussion. Setting around the table and discussion, going to the board occasionally, worked. Having a mix of engineers and ecologists, coupled with a senior professor and research assistant attending nearly every meeting of the class, provided an interesting dynamic.

Good software tools are essential for today's students. The learning curve associated with any individual package is difficult. Excel is a platform that is widely used. Students should learn a program such as MATLAB and have it used throughout the curriculum. The ECONET package herein builds off the MATLAB platform and thus is easy to grasp.

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