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Index

Control algorithms for photovoltaic inverters with battery storage for increased self consumption 1
Philipp J. Rechberger, Gerald Steinmaurer, Robert Reder

Theoretical and experimental investigation for "storage less" control of a water pumping system fed by intermittent renewable sources 7
Amine Ben Rhouma, Jamel Belhadj, Xavier Roboam

Effective use of resources in closed value networks 12
Anja-Tatjana Braun, Joerg Mandel, Thomas Bauernhansl

Electro-thermal simulation of lithium ion batteries for electric and hybrid vehicles 16
Zul Hilmi Che Daud, Daniela Chrenko, Fabien Dos Santos, El-Hassane Aglzim, Luis Le Moyne

Optimization of racing series hybrid electric vehicle using dynamic programming 23
Zainab Asus, El-Hassane Aglzim, Daniela Chrenko, Zul-Hilmi Che Daud, Luis Le Moyne

Eco-bond graphs: an energy-based modeling framework for complex dynamic systems with a focus on sustainability and embodied energy flows 33
Rodrigo D. Castro, François E. Cellier, Andreas Fischlin

Environmental performance of global supply chains observed through extended material requirements planning simulation model 46
Danijel Kovacic, Marija Bogataj

Emergy tracking – safe transition from a world of exponential growth to one of sustainability 55
François E. Cellier

Complementing life cycle assessment by integrated hybrid modeling and simulation 60
Bochao Wang, Séverin Brême, Young Moon

Policy function approximation for optimal power flow control issues 66
Stephan Hutterer, Michael Affenzeller

Simplified strategy for modeling the performance of a novel multi house heating schemes 71
John Rogers

Options for switching modes of transport in Vienna 80
Gerda Hartl, Gabriel Wurzer

Developing a sustainability assessment tool for socio-environmental systems: a case study of systems simulation and participatory modelling 83
Luisa Perez-Mujica, Terry Bossomaier, Roderick Duncan, Andrea Rawluk, Max Finlayson, Jonathon Howard

A demand response system for hierarchically organized aggregators in smart grids 92
Sergios Soursos, Vassilis Kapsalis, George Petropoulos, Yiannis Karras, Loukas Hadellis

Electricity market and renewable energy integration: an agent-based conceptual model 101
José Carlos Sousa, Zafeiris Kokkinogenis, Rosaldo Rossetti, João Tomé Saraiva

A review of control strategies for analyzing and designing managing wind generators 109
Vaia K. Gkountroumani, Peter P. Groumpos

A new generic model for greenhouses using fuzzy cognitive maps 114
Vasiliki K. Bouga, Peter P. Groumpos

Quantitative simulation of comprehensive sustainability models as game based experience for education in decision making 119
Agostino Bruzzone, Marina Massei, Simonluca Poggi, Margherita Dallorto, Giulio Franzinetti, Andrea Barbarino

Author's Index 127

ECO-BOND GRAPHS: AN ENERGY-BASED MODELING FRAMEWORK FOR COMPLEX DYNAMIC SYSTEMS WITH A FOCUS ON SUSTAINABILITY AND EMBODIED ENERGY FLOWS

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ABSTRACT
This article presents general methodology for modeling complex dynamic systems, focusing on sustainability properties that emerge from tracking energy flows.

We adopt the embodied energy (*em*ergy) concept that traces all energy transformations required for running a process. Energy can therefore be studied in terms of all energy previously invested up to the primary sources, and sustainability can be analyzed structurally.

These ideas were implemented in the bond graph framework, a modeling paradigm where variables are explicitly checked for adherence to energy conservation principles.

We introduced the new Ecological Bond Graphs (EcoBG) along with the EcoBondLib Modelica library.

EcoBG represent systems in a three-faceted fashion, describing dynamics at their mass, energy, and *em*ergy facets.

EcoBG offers a scalable formalism for the description of *em*ergy *dynamic* equations (resolving some mathematical difficulties present in their original formulation) and new capabilities for detecting unsustainable phases not automatically discovered when using the *em*ergy technique alone.

Keywords: energy, sustainability, emergy, bond graph, Modelica

1. INTRODUCTION

Modern societies rely on complex interactions with natural systems at many spatio-temporal scales. Such interactions often operate at rates exceeding the natural systems' capacity to renew (Rockström et al. 2009), leading to unsustainable structures.

As all human-driven processes depend ultimately on natural resources, their depletion, or overexploitation in case of naturally renewable ones, will necessarily shape the intensity, or even feasibility, of these processes in the future.

In order to study feasible future scenarios for human-driven processes, different approaches are required depending on the sustainability of the human´s utilization of non-renewable and renewable services and goods, notably those from ecosystems.

For this kind of analysis it may be key to take into account the whole pathway of energy transformations that human-driven processes require (e.g. notably the combustion of fossil fuels).

Means are needed to model systems and analyze the sustainability of such energy transformation paths.

A sustainable socio-natural system can be thought of as a "healthy ecosystem" (Campbell 2000). Quantitative views of ecology (Breckling, Joop, and Reuter 2011) help defining, measuring, and interpreting ecosystems' health. In his seminal textbook, E.P. Odum (1954) proposed also to quantify relations among the components of an ecosystem in a systems theoretical manner to enable ecosystem management. His brother H.T. Odum extended this idea (Odum 1983, Odum 1996) to represent related elements of ecological systems in energy equivalents, e.g. as contained in biomass (the energetic content of biomass was used as a unifying measure for universal descriptions across differing ecosystem types).

It was recognized that ecosystems have structures and functions that operate across a broad range of spatial and temporal dimensions (Allen and Starr 1982) and the overall integrity of a system, when adding human dimensions, may differ depending on the hierarchical scale at which the ecosystem is being utilized (e.g., an ecosystem supporting an industrial society may be "healthy"; however, an ecosystem receiving extensive waste from industrial processes may become "unhealthy").

A modeling approach known as Energy Systems Language (ESL) (Odum 1971, Odum 1994) was proposed to represent and analyze such systems across many spatial and temporal scales and hierarchies of organization (e.g. Allen and Hoekstra 1990).

Modeled processes should observe the laws of thermodynamics just like their physical counterparts (Odum 1996). H.T. Odum proposed that the emergence of hierarchical organization results from dissipation of the available energy (Odum 1983) and that feedback loops are created if energy is available in sufficient amounts (Odum 1988). The transfer of energy throughout a hierarchy served Odum as the basis for defining "embodied energy", or ***em*ergy**.

ESL proposes a modeling approach that represents all conceivable resources in terms of a common accounting unit. As a simple illustration, (Baral and Bakshi 2009) consider a hypothetical supply chain for a biofuel, where 1000 J of sunlight are needed to produce 10 J of biomass, which in turn are used to produce 1 J

worth of fuel. Note all those energy amounts correspond to each other and are equated by introducing some common unit. Say 1 J of biofuel is equal to 1000 solar equivalent Joules (sej). Such an approach allows for adding various further resources in terms of their solar equivalents, and the assumption of substitutability is satisfied. This approach retains information on resource quality, thereby diminishing criticism about the loss of information due to energy path aggregation (Haberl et al. 2006).

An energy quality indicator referred to as "Transformity" (Tr) converts all resources into solar equivalent joules. It has been proposed that resources with higher transformity values are of higher quality and may be scarcer (Odum 1996).

Emergy analysis is therefore of great importance as it features the unique capability of quantifying the contribution of diverse ecosystem goods and services under a common and meaningful measure, enabling a comprehensive, yet rigorous sustainability analysis.

Nevertheless, the emergy approach relies on detailed knowledge about complex socio-natural systems, which is likely to be inaccurate and incomplete. As a consequence, the method is considered controversial by some authors (Haberl et al. 2006).

Since this approach permits the modeling of flows of energy by highly non-linear functions, very complex behavior can arise. This is already the case with very simple model equations. Thereby it becomes difficult to guarantee that the resulting model is consistent with physics, i.e., that the laws of thermodynamics are not violated. However up to the present, correctness in terms of the adherence of models to physical first principles relies to a large extent on the experience of the modeler, and little assistance is provided by current modeling and simulation technologies supporting the modeler in this endeavor.

Iterative improvements or other refinement of such models by including the latest insights or by increasing resolution, often implemented over the course of several years, add particular risks. It may well be that the model is not only improved by reducing inaccuracies or removing incompleteness, but is also exacerbated by becoming thermodynamically no longer feasible.

Therefore, there arises a need for a modeling methodology that supports all of the features of ESL while guaranteeing thermodynamic feasibility.

1.1. Solutions proposed

Here we propose a new methodology that offers not only means to extend and enhance models incrementally, modularly, and hierarchically, but also provides techniques for tracking flows of matter and/or energy through the system in a systematic and rigorous way.

We present a formal system-theoretic Modeling and Simulation (M&S) framework, named Ecological Bond Graphs (EcoBG), along with a software tool that supports this novel methodology. This methodology is expected to be applicable in a flexible and efficient, yet rigorous and sound manner in M&S of complex natural and socio-economic systems, in particular when studying sustainability.

The framework consists of two pivotal cornerstones: an abstract graphical *specification layer* to work with system elements and structures (served by bond graph technology) at the top, and a specific equation *encoding level* (served by Modelica technology) at the bottom. Such an approach offers separation of the model specifications from implementation details while still aiding hierarchical modeling of target systems at all levels in an integrated manner.

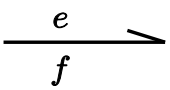
2. BACKGROUND

2.1. Bond graphs

Bond graphs (BG) (Borutzky 2010, Cellier 1991) are a multi-physics modeling paradigm intimately concerned with the conservation of energy flows. The interdisciplinary concept of energy flow creates a semantic level that allows BGs to be independent of the modeling domain. Basic concepts of physics, such as the laws of thermodynamics, can be verified in a bond graph independently of their application domain.

Three different Modelica libraries have been created for dealing with different modeling goals embracing the bond graph approach: BondLib, MultiBondLib, and ThermoBondLib.

BondLib (Cellier and Nebot 1991) makes use of the regular (black) bonds shown below.



Regular bonds carry two variables, the effort, e, and the flow, f. They do not carry units in order to make them usable for all application areas. If a bond gets connected e.g. to an electrical system, the bond inherits units of Volts for the effort variable and units of Amperes for the flow variable and propagates those units across junctions throughout the model topology.

Following this idea, complex models involving interactions among different energy domains (e.g. electrical, mechanical, and hydraulic) can be built under the same paradigm.

MultiBondLib (Zimmer and Cellier 2006) operates on (blue) multi-bonds, consisting of vectors of unit-less scalar bonds. Multi-bonds represent generalizations of regular bonds. This feature is usually needed in applications modeling 2D and 3D mechanical systems, but the concept is completely general. Here, the effort and the flow are vectors of length N that don't carry units by themselves, but inherit those later through connections to elements that belong to a particular energy domain, such as mechanics.

Whereas the dynamics of e.g. electrical or mechanical phenomena can be fully captured by pairs of power variables, thermodynamic phenomena require three independent variables for their description. ThermoBondLib (Cellier and Greifeneder 2008)

operates on (red) thermo-bonds. Contrary to the regular and multi-bond, they carry units of their own. Red thermo-bonds carry three effort variables (Temperature, Pressure, and Gibbs potential), three scalar flow variables (Entropy flow, Volume flow, and Mass flow), and also three state variables (Entropy, Volume, and Mass).

2.2. Bond graphs for sustainability analysis

In this work, we are interested in the ability of tracking flows of emergy, particularly in systems described by their mass flows. The emergy concept presents a fundamental departure from previous existing specializations of bond graphs.

Therefore, we introduced the concept of Ecological Bond Graphs (EcoBG) that operate on (green) eco-bonds. These were implemented in a fourth Modelica library, coined EcoBondLib.

As shall be discussed in detail, eco-bonds transport a single pair of power variables (just as in regular black bonds) carrying Specific Enthalpy and Mass Flow, but in addition, they also transport state information (just like in the red thermo-bonds), namely the Mass, and they also carry an information variable representing Specific Emergy. The latter will allow conducting sustainability analysis based on the embodied energy technique.

3. ENERGY CONSISTENCY AND SUSTAINABILITY ANALYSIS IN COMPLEX DYNAMIC MODELS

Our methodology focuses on models exhibiting complex dynamics. Emphasis is on structurally complex models used to study sustainability. In the following, we shall refer to these models as Complex Dynamics Sustainability Models, or CDSM for short. CDSMs are often derived from observations of the evolution of measurable variables. In the context of sustainability, the energy is key, and we therefore focus on CDSMs that describe processes by means of flows of mass and their associated energy.

CDSMs in socio-natural sciences are often impossible to be deduced from first-principle physical laws (bottom-up approach) in spite of the fact that the latter are invariably dominating any real world process. Following top-down approaches, CDSMs are built from, tuned for, and validated against real world observations, thereby gaining validity.

However, the internal structure of a model validated at the level of its observables may sometimes make questionable assumptions from an energetic point of view. Such a CDSM can be misleading in at least two ways. If the goal of the model is to *understand* the mechanisms behind a system under analysis, it may provide wrong explanations for the observed phenomena. If the goal is to *forecast* plausible future evolutions of the system, it may fail to offer credible predictions even for previously well-fitted variables.

Improving the internal energy consistency of CDSMs cannot guarantee that the model is correct, but it can at least help to rule out models that are energetically unfeasible, thus enhancing the overall model reliability.

Moreover, an energy consistent CDSM can provide novel insights about the *sustainability* of the underlying mechanisms driving the real system. By making explicit the main paths of energy transformation attached to every observable variable -including all energy sources- can point out dependencies on energy renewability constraints that might otherwise remain hidden.

4. ENERGY AND EMERGY FOR CDSM: A SYSTEM THEORETIC FORMULATION

We can abstract and generalize the modeling problem in terms of system theoretic principles, boiling it down to producing a mesh of Nodes (sources -or inputs- U, accumulators -or system states- X, and sinks -or outputs- Y) that are interlinked by Edges (physical transformation processes PR). The model is complete once we also define a system boundary to delimit our system Σ from the rest of the universe Ω (Figure 1). Linear dynamics can be expressed by defining the four system matrices A, B, C, D. Nevertheless for CDSMs, linearity is not the most usual case, and therefore we need to resort to a more general process $\dot{X} = PR(U, X, Y)$ to describe the (possibly complex) interactions among any two Nodes, similarly to what Fischlin introduced (Fischlin 1991) as the relational di-graph to define system structure using a 2nd order predicate for such a generalized process.

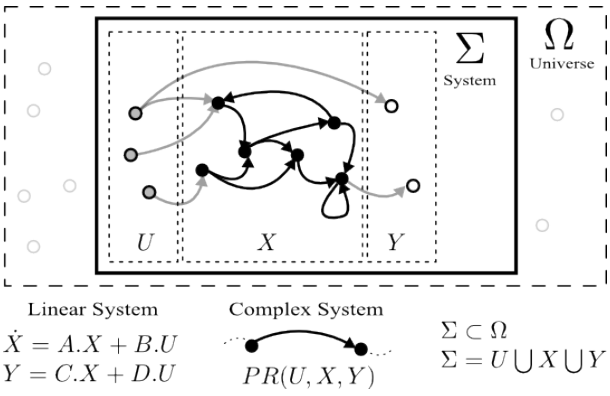


Figure 1: System-theoretic formulation of complex dynamic systems with Sources, Internal States, and Sinks.

We want each Node to express explicitly the relation between its mass and the associated energy. We shall denote the latter with H [Joule] referring to the enthalpy of the mass M[kg].

Such a relation must be consistent with the flows of energy (i.e. Power $\dot{H}$ [Watt=Joule/sec]) routed in and out through its connected Edges.

This problem is of a "local" nature in the sense that all variables required to formulate a consistent set of mass and energy equations are local to the Node and its

connected Edges. No information about other Nodes is required.

We also want to track flows of e*m*ergy[1], $\dot{EM}$ [W]. This problem, however, bears characteristics of a "structural" nature. The e*m*ergy flowing into a Node must equal the sum of e*m*ergies flowing out from its donor Nodes *regardless of the processes connecting them*.

As every real process results in dissipation of energy in the form of flows of irreversible entropy $\dot{S}_{irr}$ [W], the amount of energy actually reaching a Node will always be smaller that the energy extracted from its donor Node. Nevertheless the e*m*ergy must track the original energy required to drive the Process, i.e., *the en*ergy *used before considering losses.*

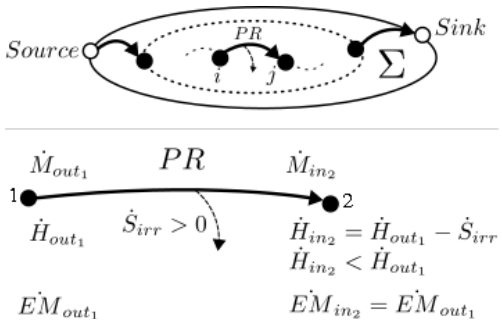


Figure 2: Process relation (PR) as the generalized Edge. Production of irreversible entropy is explicitly considered with $\dot{S}_{irr} > 0$ (2nd principle of thermodynamics).

The bottom graph of Figure 2 represents a general pair of nodes i=1,j=2. The e*m*ergy flowing into Node 2 is the e*m*ergy flowing out from Node 1, which in turn accounts for all the e*m*ergy supplied by its donor nodes[2]. When this concept is propagated across all connected pairs in a system, we realize that a change anywhere in the structure of the mesh can potentially influence the e*m*ergy of a given Node, even when its local energy balance remains intact.

1 Flows of emergy are also referred to as Empower in the emergy literature.

[2] H.T.Odum's original formulation for ĖṀ resorts to a set of differential equations that are switched depending on the dynamics of the energy at a Node: increasing, decreasing or steady state (Odum 1996) These were termed "differential-logic equations" for "Dynamic Emergy Accounting – DEA." Strictly speaking, it consisted of a piecewise continuous type of system with discontinuities triggered by state events. As we shall see later, by sticking to our BG-based methods, we are driven to reject this switching idea, obtaining a more physically sound formulation for ĖṀ. Tilley reached the same conclusions following other rationales (Tilley 2011). The two approaches were developed in parallel and independently of each other (Castro and Tilley 2012, personal communication).

E*m*ergy captures a system property sensitive to its structure by memorizing energy supplies back to the sources at the system's boundary.

At a given node, the Transformity $Tr = \frac{EM}{H}$ denotes the proportion between the e*m*ergy (EM) sustaining all previous paths of transformations (leading to the existence of that node) and the locally usable energy (H). For a given H, a higher Tr implies chains of energetically less efficient transformations, the system having to invest more energy at its sources.

4.1. A Multi-Faceted Approach

In accordance with the system-theoretic framework developed above, we propose a compact view of Nodes and Edges decomposed into three facets: a "Mass Facet," where the local laws derived from observations are encoded, and two energy-oriented facets, namely the "Energy Facet" and the "E*m*ergy Facet" (of local and structural nature, respectively), as depicted in Figure 3.

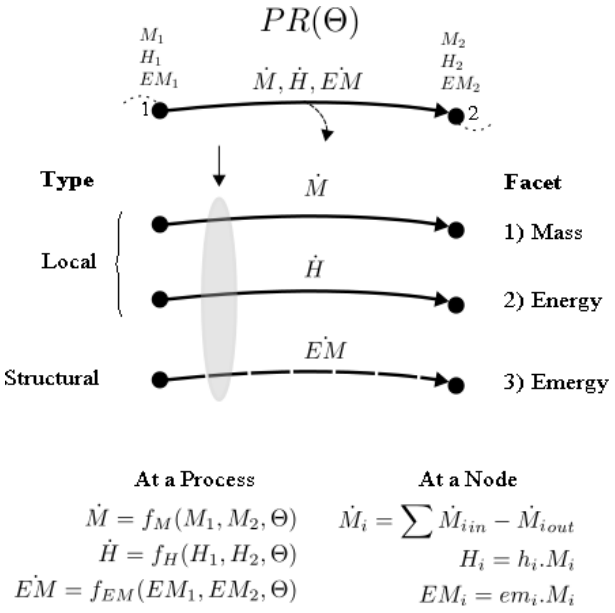


Figure 3:Three-faceted view (Mass, Energy, and Emergy) of the generalized process **PR**(**Θ**). **Θ** is a parameter vector.

All Nodes and Edges are then equipped with mass-, energy- and e*m*ergy-awareness. This separation of concerns helps us to obtain a compact core set of equations for expressing CDSMs that is capable of scaling up for defining complex systems in a robust way.

It also fosters easy assimilation of techniques other than e*m*ergy tracking to account for past energy transformations while keeping equations in the mass and energy facets encapsulated and self-consistent.

5. BOND GRAPHS AS THE ENERGY-BASED PRACTICAL MODELING PARADIGM

We shall now map the systemic approach of the previous section into a practical modeling formalism.

As illustrated in Section 2.1, BGs offer a highly suitable modeling framework for the purposes at hand: BGs natively distinguish between structure and behavior, are based on the explicit tracking of energy flows (expressed by their basic pairs of *effort* and *flow* variables), and enforce energy conservation laws.

As already conveyed in Section 2.2, we shall define a new core set of BG elements suitable for building CDSMs including e*m*ergy tracking capabilities. We shall refer to those as "Ecological Bond Graphs," or EcoBG for short. We shall proceed guided by motivating examples of increasing complexity.

5.1. Motivating Example 1: Source-Storage-Sink

This first example is inspired by a frequently referenced model proposed by H.T. Odum (1996) named EMTANK (E*m*ergy Tank), a classical starting point for e*m*ergy methodology. It represents the most basic case possible from a structural point of view, as one single node "Storage" has connections only to system boundaries, and from a dynamical point of view, because processes from/to sources/sinks are simpler to model than processes linking storages.

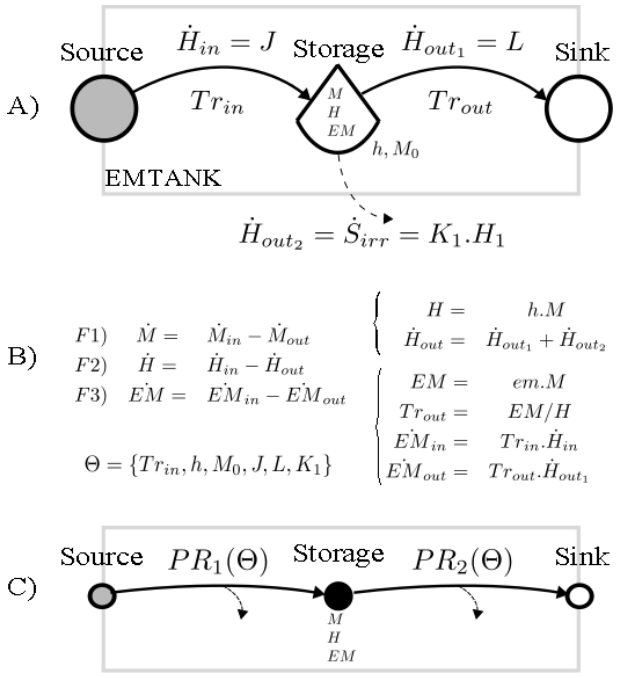


Figure 4: The EMTANK system. A) Original ESL formulation, B) Three-faceted view, and C) System-theoretic formulation.

Some considerations are in order. In Figure 4A, the dynamics of the original model are expressed directly in terms of flows of energy ($\dot{H}$) rather than flows of mass. In our approach, we can mimic this by setting the specific enthalpy to $h = 1$ J/kg, thus operating on generic masses. The equations of Facet 1 and Facet 2 look the same and deliver identical numerical values, albeit using different measurement units.

For the e*m*ergy equations (Facet 3), we can assume $E\dot{M}_{in} = \dot{H}_{in}$ by setting $Tr_{in} = 1$. A Source Node is a special case as it may import e*m*ergy flows from other subsystems, and Tr_{in} is the way of encoding it. Also, different Tr values can be used to scale flows of different types of energy in such a way that they are "converted" to flows of a single chosen type.

In Figure 4C, we mapped the example to our graph-like system-theoretic formulation.

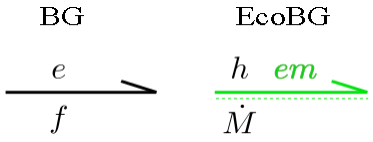
5.2. The EcoBG Bond element

The basic BG element that transports energy between elements is the bond.

The most suitable pair of variables for CDSMs is that formed by the specific enthalpy h (an *effort variable*) and the mass flow $\dot{M}$ (a *flow variable*). Hence $\dot{H}$ [J/sec] = h [J/kg] · $\dot{M}$ [kg/sec] represents power [W=J/sec], i.e., flow of energy.

While h and $\dot{M}$ provide enough information for depicting equations of Facets 1 and 2, we need additional information for Facet 3, i.e., the e*m*ergy facet. We thus add to our bond the specific e*m*ergy *em* [J/kg] as an *information variable*, whereby $E\dot{M}$ [J/sec] = *em* [J/kg] · $\dot{M}$ [kg/sec] also denotes flow of energy.

The reason for choosing the *information* type rather than the apparently more suitable *effort* type for *em* will become evident later on. We shall represent EcoBGs with the classical harpoon with an extra dashed line indicating that information variables are being included.

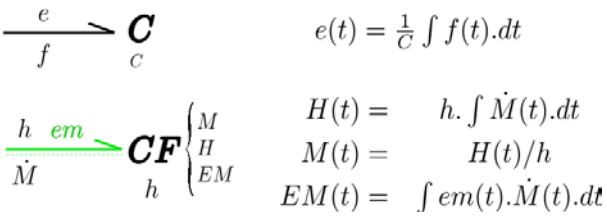


In the Modelica implementation of the EcoBG methodology, i.e., in the EcoBondLib Modelica library, we color-coded the new EcoBG bonds (eco-bonds) using the green color.

5.3. The EcoBG Mass Storage element

We made it already clear that our approach is particularly concerned with processes transporting and transforming mass, as well as storage elements for accumulating mass.

The type of BG element suitable for mass storage is the C-element (or capacitor), as by definition, a C element integrates the flow variable and calculates the effort variable.



As we can see, the parameter C of the mass storage element must be $C = 1/h$. This is consistent with the idea that storages in a model represent *one particular*

type of mass that can be uniquely characterized by its specific enthalpy.

The EcoBG C must also integrate e*m*ergy. To that end it resorts to em, the specific e*m*ergy information attached to the mass flow $\dot{M}$. In this case however, there does not exist a constant specific e*m*ergy characterizing the mass, as it is a consequence of chains of processes taking place somewhere else in the topology. Therefore $em = em(t)$ is kept inside the integral.

5.4. The EcoBG Junction element

Junctions in BGs are structural elements enforcing e*n*ergy *conservation* among those elements interconnected via the junction through their bonds.

0-Junctions achieve that goal by enforcing *flow conservation* while operating at a common effort. 1-Junctions enforce *effort conservation* among components operating under a common flow.

As systems described by mass flows are the primary objects to be captured by EcoBG models, the 0-Junction is the suitable element to be extended to cope with the concept of e*m*ergy.

The EcoBG 0-Junction element distributes a common specific enthalpy among its connected bonds, and enforces mass conservation through $\sum \dot{M} = 0$ (cf. Figure 5). When a storage is connected to a 0-Junction, C becomes the element imposing its specific enthalpy h to the other connected bonds.

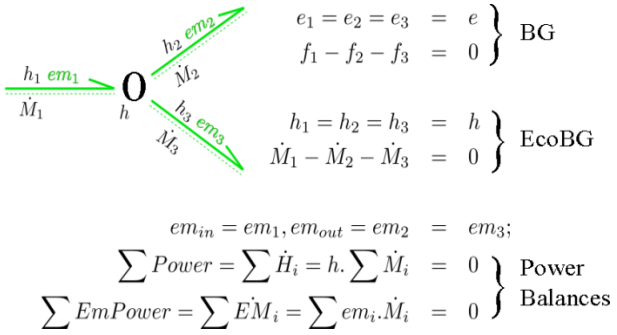
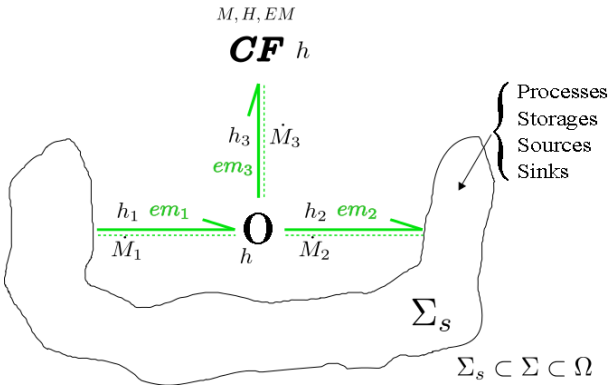


Figure 5: The EcoBG 0-Junction. Balances of Mass, Power, and EmPower.

In Figure 5, the e*m*ergy balance looks different from the power balance represented by $\sum h.\dot{M} = 0$, as there is no em common to all flows. According to the e*m*ergy principle, incoming flows contribute their own values of e*m*ergy per unit mass to build and sustain the storage, while all outgoing flows bear a new and common value of specific e*m*ergy imposed by the storage. This explains why we treat em as an information variable rather than as an effort variable.

We can now take a look at a basic unit composed by the EcoBG elements defined so far, which will serve as an important building block for more complex models.



With the proposed variables, we are now able to describe the storage of mass while adhering to the multi-faceted approach proposed in Section 4.1.

5.5. EcoBG Process elements

So far we described the basic tools needed to make Nodes connectable to the rest of the system while observing basic conservation principles. We still lack an element where to encapsulate the relations connecting Nodes. This will be our Process element that populates the Edges webbing our topology. A Process shall encapsulate two fundamental pieces of information:

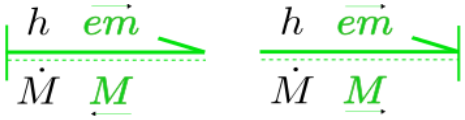
Firstly at the Mass Facet, it describes the laws relating masses. The most general dynamic formulation for defining relations among masses looks as follows:

$$\begin{cases} \dot{M}_1 = f_1\,(M_1, \dots, M_n) \\ \quad \vdots \\ \dot{M}_n = f_n\,(M_1, \dots, M_n) \end{cases} \quad \textbf{(1)}$$

In our motivating example, we have only one type of mass, and assuming $h = 1$ for the sake of simplicity, the Process must express:

$$\begin{cases} \dot{M}_1 = J - K_1.M - L \\ H = h.M, h = 1 \end{cases} \quad \textbf{(2)}$$

For a Process element to be able to calculate $\dot{M}_1 = -K_1.M$, it needs to know the value of M, which so far is a variable internal to the C element. Therefore, we need to extend our bond element with one additional information variable carrying M, i.e., the *state* of the accumulated mass at the storage. Just like h, this variable can only be imposed by a C element.



Secondly at the Energy Facet, Processes shall be responsible for encoding the loss of energy due to production of irreversible entropy, an inevitable feature of all real processes.

The consequence of the latter for the E*m*ergy Facet is evident: the information of the energy used *before* the

discounting of irreversible entropy shall be passed along unaltered for the emergy accounting purposes already discussed.

In Example 1, the two required Processes are special ones -in fact, the simplest possible- due to Source and Sink being special types of Nodes. These Nodes' mass and energy balances are unidirectional as they only impose or accept power flows, respectively. They are placed at the system's border, and they don't accumulate mass or energy.

We shall first define the Source Process and the Sink Process. At a later example, we shall deal with the more general type of Process interconnecting Storage Nodes among themselves.

5.5.1. The EcoBG Source Process

We must derive a structure to represent "Process 1" in Figure 4C.

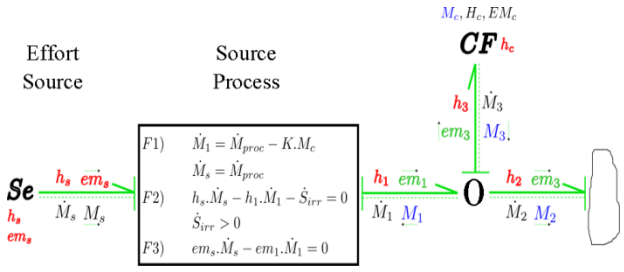


Figure 6: The Source Process

Facet 1 (Mass Facet). The EcoBG Source Process (Psrc) element provides the flow of mass injected into the Storage (after losses).

An EcoBG Effort Source (Se) element must feed Psrc with the energy associated with the demanded mass flow in the form of specific enthalpy (before losses).

Eq.(F_1) expresses the laws for the mass flows considering that the mass brought in from the Source ($\dot{M}_S$) is configured as a *parameter of the process* ($\dot{M}_{proc}$) by the user and taking into account the mass lost due to the generation of entropy ($K.Mc$). The mass flow is imposed by Psrc to Se ($\dot{M}_S = \dot{M}_{proc}$), as we adopted mass flow, rather than energy flow, as the main flow describing the dynamics of the system.

Facet 2 (Energy Facet). The flow of energy entering Psrc must equal the flow of energy carried by the mass entering the Storage plus the flow of energy dissipated as entropy ($\dot{S}_{irr}$).

The specific enthalpy is imposed at the right hand side of Psrc by the Storage element ($h_1 = h_c$).

Under normal circumstances, the user-provided parameters h_S and h_C should match, as the type of substance being supplied by Se and subsequently accumulated in C is of the same type. Yet, these parameter values can be chosen differently. The energy balance would then absorb the disparity with the additional capability of checking whether this generates physical inconsistencies (i.e., $\dot{S}_{irr} > 0$ must always hold). An h_S greater that h_C can be used to represent the energy required to procure the mass from the rest of the system (e.g., to extract a mineral from its ore).

Facet 3 (Emergy Facet). The specific emergy em_S supplied by the Se element can be set as a parameter by the user. Emergy flow reaches Psrc to the amount of $E\dot{M}_S = em_S.\dot{M}_S$. This emergy flow is propagated unaltered to the right hand side of Psrc as $E\dot{M}_1 = em_1.\dot{M}_1 = E\dot{M}_S$, ignoring the irreversible loss of energy via $\dot{S}_{irr}$ (in accordance with the principle of emergy accounting).

5.5.2. The EcoBG Sink Process element

Following a similar approach, we shall derive the structure to represent "Process 2" in Figure 4C. In fact, we can already take advantage of the systematic formulations made so far and make the Sink Process be just a mirror version of the Source Process.

Conceptually, we should be able to simply invert the signs of flow equations in Facets 1, 2, and 3, thus transforming inputs to outputs, and vice-versa. In BGs, such an idea is achieved by inverting the bonds' harpoons that indicate the direction of positive flows (cf. Figure 6).

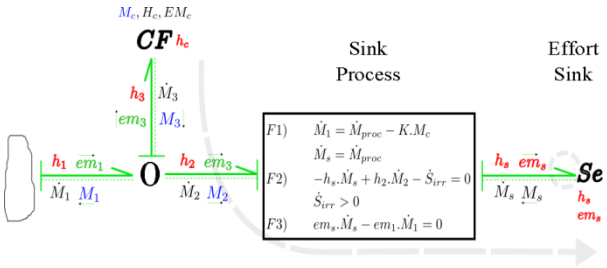


Figure 7: The Sink Process

In Figure 7, we see the schematic representation of this idea. The Sink Process (Psnk) element defines through its phenomenological law, how mass is extracted from C.

The Se element (a source of effort now operating as a Sink) can state the energy required for taking the mass out of the C element (h_S) together with the emergy associated with that energy (em_S).

However, these parameters will not have any influence on the rest of the model: the energy contained per unit mass in C is defined by h_C, and its emergy per unit mass is calculated as $em_C = \frac{EM_C}{M_C}$ also at the storage element. Yet, specifying h_S and em_S can serve for the comprehensiveness of the model as a whole.

5.6. The EcoBG EMTANK Model

We already defined all of the EcoBG elements required for representing the model of Figure 4.

The next figure shows the coupling of elements achieving that goal.

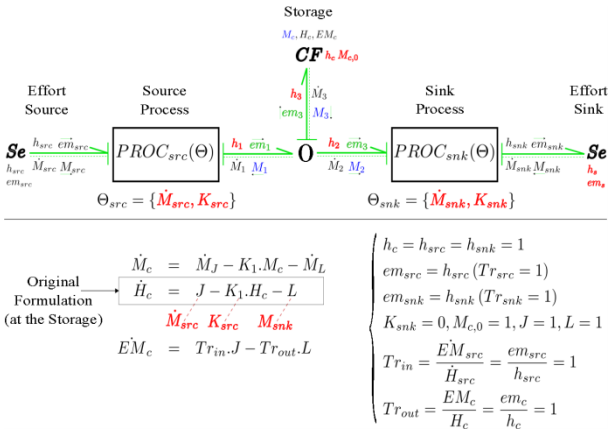


Figure 8: The Source-Storage-Sink system (EMTANK).

In the lower part of Figure 8, we can see the equations that are automatically extracted from the graphical model by the Modelica compiler. We set the specific enthalpies and emergies to 1 for the sake of simplicity while analyzing the first results.

At Facet 2, we see that parameter K_{snk} of process Psnk plays no role, as we set $K_{snk} = 0$, implying that the process of mass/energy consumption from the Storage considers no losses. On purpose, we decided to assign all losses due to entropy generation in the original model to process Psrc.

In Odum's ESL language, dissipation losses can be modeled at Storages and/or Processes, with the former option being the one usually adopted. In ESL, dissipation losses represent emergy-less processes on their own. Nevertheless in the EcoBG approach, we consider that losses exist only as consequences of mass transformations (i.e., processes), and therefore the correct place to model them is at the EcoBG PROC elements.

At Facet 3, we recognize that the term $K_{src}.M_C$, present at Facets 1 and 2, takes no effect. This is because in EMTANK, this is the flux meant to describe irreversible losses, therefore carrying no emergy. For this reason, it must not be subtracted for emergy accounting.

5.6.1. Model Implementation

We implemented the EcoBG elements introduced so far as individual models encoded in the Modelica language (Modelica 2013a)

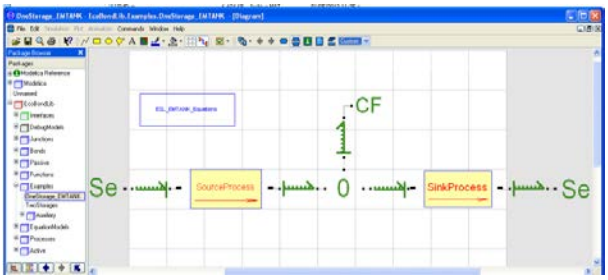


Figure 9: The EcoBG implementation of the Source-Storage-Sink system in Dymola.

In particular, we used the Dymola visual modeling and simulation environment (Dymola 2013). We shall delve more into the implications of this approach in Section 7.

Figure 9 shows EMTANK implemented in the Model view of Dymola.

Besides implementing the EcoBG version of EMTANK, we encoded a subsystem capturing the original set of equations defining EMTANK for comparison purposes (cf. the blue box in Figure 9). Parameter values were set for each element according to those presented in Figure 8.

5.6.2. Model Simulation

We simulated the model for t_f=350 units of time, i.e., until steady state is reached.

The next Figure shows the results for the main variables of interest: M, H, EM and Tr simulated at the Storage element in the EcoBG model and also at the EMTANK block that implements the standard equations proposed by Odum (legends squared with dotted lines).

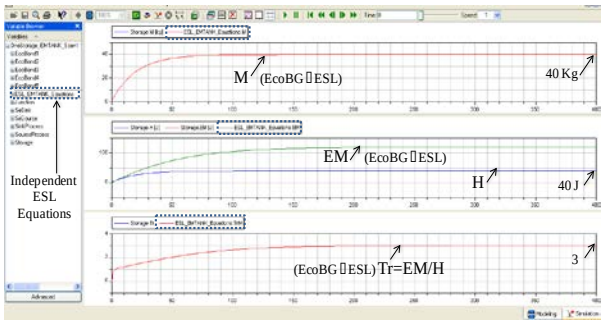


Figure 10: Baseline simulation of EMTANK with EcoBG and standard ESL equations. EcoBG mimics ESL results.

We verify that the EcoBG model mimics exactly the original EMTANK behavior (the trajectories are indistinguishable for M, EM, and Tr). We also display H together with EM. Since all specific enthalpy values were set to 1, the curve of H matches that of M. Yet H differs from EM as the latter remembers all of the energy that was used at the source before discounting losses. The ratio $Tr = EM/H$ is verified to be consistent throughout the simulation. With the given parameter values, the "quality" of each unit of mass available for consumption from the Storage at steady state is 3. In less trivial networks of processes, this number helps to identify, which Storages bear higher energetic quality, indicating that their overall energetic cost is higher.

We can now experiment with different parameter values. E.g. if we change the specific enthalpy of the mass, we should see no changes in the mass dynamics, but we should notice changes in the energy dynamics.

To do so, we set $h_C = h_S = 2$, and also $em_S = h_S$ so as not to incur changes in the transformity. Results are shown in the next figure.

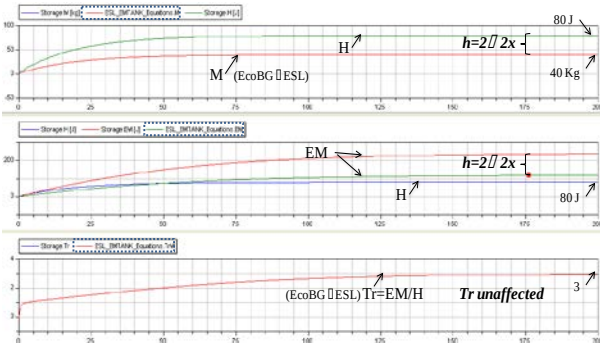


Figure 11: Scenario 1: Baseline with doubled specific enthalpy

All results are as expected. If we now change only the specific e*m*ergy at the source, making it e.g. $em_S = 2.h_S = 4$, we should see the dynamics of mass and energy unchanged, whereas now the e*m*ergy flows change by a factor of 2. This is shown and verified in Figure 12.

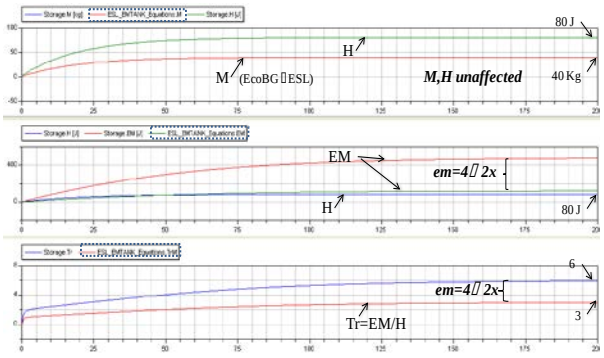


Figure 12: Scenario 2: Scenario 1 with doubled specific emergy

Before coding a less trivial example, an important remark is in order. As discussed before, we use Source elements at the systems' borders. So far we used effort sources, which state how much energy and e*m*ergy the requested mass flow shall carry. Yet we know that physical processes are always limited in terms of the maximum power they can deliver. Apparently our ideal sources are able to withstand flows of infinite energy, which is certainly non-physical.

To remedy this situation, we equip Sources with a P_{max} parameter. Should the condition $P_{src}(t) = \dot{H}(t) > P_{max}$ become true, the simulation should stop indicating that the system is requesting more power from the source than can be delivered.

P_{max} represents a coarse-grained abstraction, an assumption made for representing limitations that arise from more complex dynamics at a part of the system that has been lumped together in a single Source element.

In the next example we shall see richer dynamics by replacing the source of effort at the supply side with a submodel that accounts for flow, power, and storage limitations, representing more realistically limitations as they are found in nature.

6. EXAMPLE 2: TWO STORAGES. REPLACING IDEALIZED SOURCES. CHECKING FOR SUSTAINABILITY.

In Figure 13 we show an example that considers a natural process that produces a primary renewable reservoir of matter (C_a), which serves as the actual repository that the Supply Process at the right feeds from.

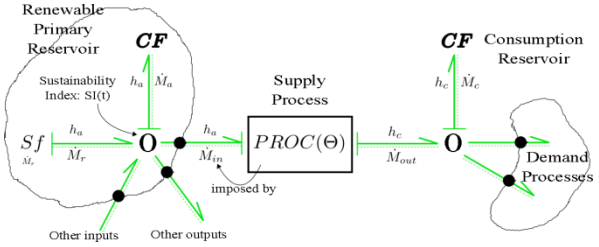


Figure 13: System with two storages: Source deposit (left) and a Consumption reservoir (right).

Now, we use a Source of Flow (Sf) element. Such a source imposes $\dot{M}_r$ while accepting the specific enthalpy imposed by the system it is connected to (in our example h_a, a parameter of C_a).

For Sf, the contributed mass flow is not a consequence of a process demanding material, but rather a known supply parameter. It represents a natural process, whose mass flow can be directly measured (such as the flow of rain filling an underground aquifer).

In this new model, the power limitation will be given by the balance between incoming and outgoing flows at the junction element. Consuming processes that draw more power than that supplied by the donor processes are not sustainable, and checks must be performed for those cases in the same way that we used to check against $P_S > P_{max}$ in our previous example.

We now talk about checking for sustainability instead for instantaneous maximum power, because processes can potentially -though only temporarily- draw more power than is being instantaneously provided by consuming the additional energy from the storage, thereby lowering its level.

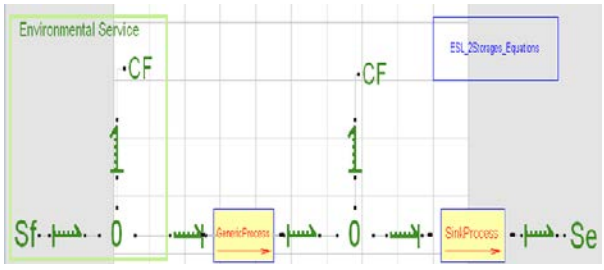


Figure 14: The EcoBG implementation of the Two Storages system in Dymola.

Parameterization for the system in Figures 13 and 14 is as follows:

$$\begin{cases} Rain\ (Sf_r)\colon \dot{M}_r = 2, h_r = em_r = 1 \\ Deposit(C_a)\colon h_a = 1, M_{a,0} = 150 \\ Supply(PR_s)\colon K_s = 0.001, K_s^{irr} = 0.1 \\ Consumption(C_c)\colon h_c = 1, M_{c,0} = 1 \\ Demand(Se_a)\colon K_d = 0.05, K_d^{irr} = 0 \end{cases} \quad \textbf{(3)}$$

The equivalent set of equations expressed with the ESL method, taking $M_1 = M_a, M_2 = M_c$ are:

$$\begin{cases} \dot{M}_1 = J - K_1.M_1.M_2 \\ \dot{M}_2 = \quad K_1.M_1.M_2 - K_2.M_2 - L \end{cases} \quad \textbf{(4)}$$

$$\begin{cases} E\dot{M}_1 = Tr_J.J - Tr_{M1}.K_1.M_1.M_2 \\ E\dot{M}_2 = \quad Tr_{M1}.K_1.M_1.M_2 - Tr_{M2}.L \end{cases} \quad \textbf{(5)}$$

Parameterization for Eqs. (4) and (5) is as follows: $J = 2, K_1 = 0.001, K_2 = 0.1, L = 0.05, Tr_J = 1$ with initial conditions $M_{1,0} = 150, M_{2,0} = 1, EM_{1,0} = EM_{2,0} = 0$.

6.1.1. Simulations

The next figure shows simulation results for a system configuration yielding oscillatory behavior (a mode possible only with 2 or more storages).

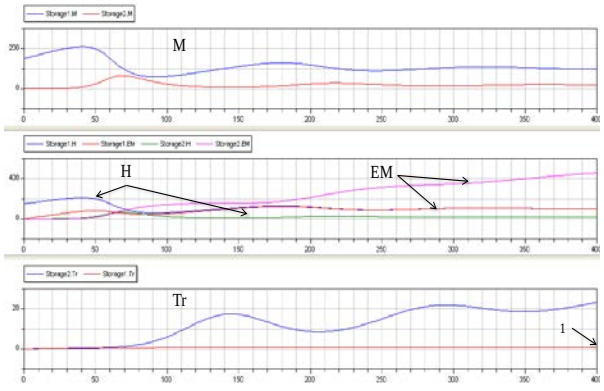


Figure 15: Baseline simulation of the Two Storages model with EcoBG.

All curves overlap those produced by an independent simulation of the corresponding ESL Eqs. (**4**) and (**5**).

For both storages, the upper graph shows M, the center graph depicts H and EM, and the lower graph displays T_r. All variables reach steady state in the long run (the oscillations die out). We can see how the non-intuitive evolution of H and EM at the second storage produces an oscillatory trajectory for its transformity, indicating that the "quality" measure as defined in the *em*ergy methodology is indeed a dynamic concept.

E*m*ergy analysis uses flows of e*m*ergy and their transformities along with labels assigned to flows (e.g. "renewable" or "non-renewable"), and then produces several sustainability-related performance indicators.

EcoBondLib provides us with all elements that we require to model and simulate the dynamics of arbitrarily interlinked storage/mass flow systems. Special indicators can be programmed easily to warn us when the simulation enters an operational mode that is not physically feasible.

6.1.2. The Sustainability Index

We shall introduce now a Sustainability Index (SI) indicator for EcoBG.

As mentioned at the beginning of the section, a sustainable balance of power must be observed locally at every source or storage, otherwise the whole system is unsustainable.

For EcoBG Junctions we define:

$$SI(t) = Power_{in}(\mathrm{t})/Power_{out}(t) - 1$$

$SI(t) < 0$ indicates an unsustainable phase, whereas $SI(t) >= 0$ denotes a sustainable phase, $SI(t)$ being the consequence of the (possibly many) simultaneous flows of energy entering and leaving the Junction. The power balance mandates that:

$$Power_{in}(t) - Power_{storage}(t) - Power_{out}(t) = 0$$

For $SI(t)$, we ignore $Power_{storage}(t)$, i.e., how much power is being accumulated by or consumed from the storage, because the condition $Power_{out}(t) > Power_{in}(t)$ is unsustainable regardless of the behavior of the storage.

At a Source, we set $Power_{in}(t) = P_{max}$ (a parameter of the element). Therefore, SI(t) will depend solely on the $Power_{out}(t)$ imposed from the connected processes.

This sustainability concept, local to nodes in a system, is not present in ESL and is not a matter to be captured at the e*m*ergy facet[3].

In the next figure, we show the results of a scenario where we reduced by a factor of four the constant inflow of mass supplied by nature (rain) into the renewable storage (aquifer, C_a). The figure presents the impact of this change on the second storage (consumption, C_c).

[3] An E*m*ergy Sustainability Index (ESI) exists that depends in turn on other e*m*ergy-based indices relying on qualitative tagging. While e*m*ergy-based indices are a useful tool, they are of a relative nature: they depend on arbitrary choices made for e.g. the tagging procedure or the system boundary definition. In contrast, our SI indicator is based on energy, and is locally unambiguous for each junction where it is evaluated, regardless of assumptions made elsewhere.

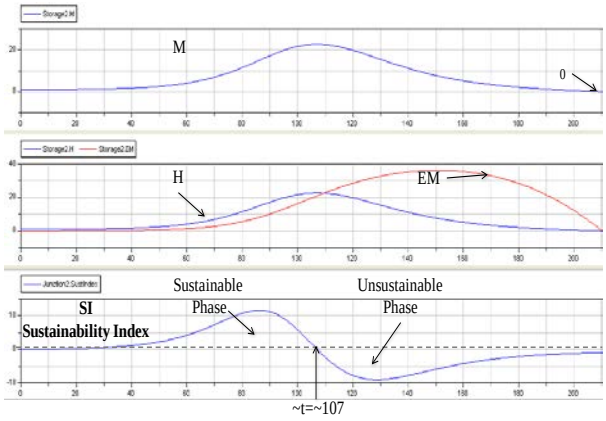


Figure 16: Scenario 1: Baseline with natural inflow reduced by four. Curves are for the second storage.

Contrary to the baseline scenario where we decided to finish the simulation at t_f=400, the simulation stops at t_f=210 in this second scenario, because C_c gets emptied and cannot supply anymore the demanded flow of energy.

In the bottom panel of Figure 16, we plotted SI(t). We can see that for times t_f>107 sec., SI(t) assumes negative values indicating the beginning of an unsustainable phase. The simulation never recovers from this unsustainable operational mode leading to the total depletion of C_c before its donor process can replenish it drawing from C_a. Of course, it can happen that a system experiences temporary phases of unsustainable operation from which it subsequently recovers. Such temporary unsustainable regions should be a reason for concern, but may be acceptable if no better alternative can be found.

$SI(t) < 0$ is an indication of an *instantaneous* mode of operation that *cannot be sustained forever*. This information is not intuitive and cannot be immediately derived from observing independently any of the main variables analyzed so far in any of the three facets considered.

A potential advantage of this indicator is that it can be propagated locally from a Junction to all its connected processes, opening up the possibility of designing rules of decisions to be made by processes reacting to this new knowledge. For example, the process drawing from storage C_a could shut down for a while when the storage level of C_a becomes too low, thereby granting the source enough time to replenish the storage.

7. MODELICA AS THE MODEL ENCODING LANGUAGE

We took advantage of the BG modeling framework as the foundation onto which to build and extend ideas of energy- and e*m*ergy-oriented modeling of CDSMs.

We implemented the core set of EcoBG models in Dymola, a Modelica-based modeling and simulation environment.

There are further relevant implications of having chosen this path.

7.1.1. Modeling aspects

Rather than being a traditional sequential programming language, Modelica is a mathematical modeling language that expresses mathematical relations using an object-oriented declarative textual (eventually also graphically rich) interface. A Modelica compiler checks not only for syntax errors or code completeness, but most importantly also for soundness and solvability of the set of mathematical equations encoded in the model.

Modelica features also model inheritance capabilities that make model development efficient and robust. For example, the Process models used in our examples differ in their laws governing mass and energy, but they all follow the same rule at the emergy facet (namely, they all pass along the emergy flow from input to output). This facet can then be coded once in a base "template" Process model, so that every new specialized process will inherit this functionality. Changes in the template Process will then be automatically inherited by all models that are based on that template, while retaining their specializations.

Benefitting from the latter, full subsystems can also be declared as new self-contained classes hiding away inner intricacies, exposing only selected input and output interfaces, and assigning them with convenient graphical decorators. This feature would make it straightforward to build a library of e*m*ergy models following Odum's ESL iconography while actually building them using EcoBG as the underlying plumbing technology.

Also very important for productivity, teamwork, and scientific communication, Modelica models are self documentable.

7.1.2. Simulation aspects

Modelica models can be run by any tool adhering to the language specification, which is open and standardized.

Advanced Modelica implementations, such as Dymola, offer robust integration algorithms for simulating models that are potentially difficult to deal with, such as models with a high degree of stiffness and/or heavy discontinuities. Most of the classical ESL implementations are rather weak in this respect, offering e.g. only a fixed-step Forward Euler algorithm as their simulation engine.

The dangers of relying on only one (or a reduced set of entry-level) solvers can be high. Dynamic models of even low complexity can already present serious numerical difficulties[4]. Hence drawing conclusions about sustainability issues in CDSMs by trusting outcomes of simulations tested with only one primitive numerical method is not recommended.

In this same context, having a mathematical encoding language that allows a piece of code to be

[4] E.g. a simple second-order model, such as a predator-prey model, whose trajectory solution is known to enter a stable oscillation (i.e., it exhibits a limit-cycle solution) can end up showing unstable behavior if a too large step size is chosen.

interpreted by different tools with different strengths is a considerable advantage, as models can gain more credibility and acceptance in a potentially wider community of users.

The clean separation between the modeling aspects and the simulation aspects embraced by Modelica offers an important advantage of our approach in the analysis of complex systems.

8. CONCLUSIONS

We presented EcoBG, a novel energy-based modeling framework for complex dynamic systems with a focus on sustainability and e*m*ergy flows.

By tracking simultaneously flows of mass and their attached specific enthalpy and e*m*ergy, EcoBG can check for the thermodynamic feasibility of the models, pinpointing physically unfeasible phases that cannot be detected in advance via static inspections of the model's definition.

EcoBG offers a low-level, domain-independent plumbing technology useful for building higher-level components tailored for specific application domains or modeling communities.

EcoBG was specifically designed with generality and scalability in mind. Models of increasing complexity can be built hierarchically while preserving all energy self-checking features. With EcoBG we offer a sound framework into which to embed the basic ideas behind e*m*ergy tracking, naturally lending to a mathematical formulation of emergy dynamics that circumvents the physically awkward original proposition of switching differential equations.

Although not demonstrated in this article, also available in EcoBG is the ability to simulate models with only partial knowledge about the specific enthalpy values associated with flows of masses. By only stating specific enthalpy values at sources, EcoBG will automatically choose values for unknown specific enthalpy values throughout the inner system that do not violate energy conservation principles. This can be very helpful at the early exploratory stages of a modeling process.

An EcoBG model can also be connected with other types of Modelica models. This makes it possible to mix sustainability models with other model types based on first principles in different physical domains (e.g. mechanic, electric, hydraulic, etc.) drawing from the Modelica Standard Library (MSL) (Modelica 2013b), which offers a rich palette of sophisticated models covering many physical phenomena from a wide range of energy domains.

Also benefitting from the Modelica underlying technologies, a wealth of optimization/automatic control techniques becomes easily accessible and applicable in EcoBG. An example of this could be designing processes that self-adapt their consumption/production rates according to (possibly sophisticated combinations of) dynamically calculated sustainability indices.

This is very appealing for studying sustainability of systems involving interactions between natural and industrial processes, as for the latter we can readily inherit a vast knowledge base of models developed within the Modelica community over many years.

9. NEXT STEPS

We are still one important step away from claiming EcoBG to be a full-fledged technology in terms of its emergy accounting capabilities.

There exist definite rules, called Emergy Algebra (Brown and Herendeen 1996) to assign e*m*ergy to flows of energy in special situations, such as e.g. a process generating more than one output (by-products), an output being split after it left a process (flow splits), etc. Among these, the most relevant in our view is the rule stating that emergy shall not be counted twice when recirculating through a process that it had passed through already once after completing a feedback loop - e.g. material recycling-.

In EcoBG, we are currently forced to manually deactivate the emergy carried by flows passing through a feedback loop. This implies that the user needs to detect in advance all looping flows, an approach that is clearly error prone (or even unfeasible when the size of the system grows). Yet, human-assisted approaches to feedback loops are the de facto norm in most ESL implementations today (with the EmSim simulator (Valyi and Ortega 2004) being an exception to the rule). We shall make EcoBG capable of dealing with automated loop detection rules in the next version of the formalism. We shall also supply a richer set of higher-level customized models, in particular PROC elements implementing well known functional relationships in sustainability science.

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