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An Emergent Nonlinear Thermodynamic Energy-Flow Model for Collections of Coupled Oscillators

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Abstract— **This paper investigates the emergence of thermodynamic energy flow for collections of coupled oscillators. Unlike previous work based on averaging over stochastic forcing, a stochastic model ensemble, or time, thermodynamic energy flow is viewed as a deterministic physical phenomenon arising solely due to dimension and thus consistent with the physically observed laws of thermodynamics. For two collections of undamped coupled oscillators, the kinetic and potential energy of the respective subsystems is shown to exhibit pointwise-in-time thermodynamic energy flow before energy reversal begins. However, the rate of energy flow is found to be inconsistent with the classical exponential profile corresponding to Newton's law of cooling, whose dynamics are linear. Instead, the rate of energy flow is shown to be captured by a thermodynamic energy-flow model with quadratically nonlinear dynamics.**

I. Introduction

The laws of thermodynamics are among the foundational physics underlying modern science and technology [1]. These laws are macroscopic in the sense that they are statistically valid for a large number of molecules [2]. In recent years, there has been increasing interest in recasting the laws of thermodynamics in terms of dynamical systems theory [3].

The laws of thermodynamics can be viewed as emergent properties of dynamical systems of extremely high dimension, where each molecule can be viewed as an oscillator that possesses kinetic and potential energy. This emergence is far from trivial since the classical laws of dynamics are time-reversible, whereas the laws of thermodynamics are not [3]. A longstanding research challenge is thus to demonstrate this emergence, beginning with the classical laws of dynamics applied to individual molecules.

A consequence of the laws of thermodynamics is Newton's law of cooling, which states that the rate of energy transfer between two bodies is proportional to their temperature difference [4, pp. 6, 7]. This law is given by

$$\dot{T}_1(t) = \alpha(T_2(t) - T_1(t)), \tag{1}$$

$$\dot{T}_2(t) = \alpha(T_1(t) - T_2(t)), \tag{2}$$

where T_1 and T_2 are the temperatures of Body 1 and Body 2, respectively, and α is the heat transfer coefficient. It follows from (1) and (2) that T_1 and T_2 are given by

$$T_1(t) = \frac{T_1(0) - T_2(0)}{2} e^{-2\alpha t} + \frac{T_1(0) + T_2(0)}{2}, \tag{3}$$

$$T_2(t) = \frac{T_2(0) - T_1(0)}{2} e^{-2\alpha t} + \frac{T_1(0) + T_2(0)}{2}. \tag{4}$$

Note that both temperatures converge monotonically and exponentially to the same equilibrium value, namely, $\frac{T_1(0)+T_2(0)}{2}$, which depends on the initial heat distribution. This emergent behavior constitutes thermodynamic energy flow. Compartmental models of the form (3), (4) can be used to formulate the laws of thermodynamics, as shown in [3], [5], [6].

The accuracy of Newton's law of cooling depends on the variation of the heat transfer coefficients with temperature. Consequently, this law is considered to be more accurate for conductive heat transfer than for convective and radiative heat transfer. Extensions to the latter cases are considered in [7].

One approach to understanding the emergence of thermodynamic energy flow is to average the energy flow between a pair of oscillators over the probability density of broadband random forcing; alternatively, the rate of energy flow can be averaged over an ensemble of parameters. The resulting rate of energy flow is proportional to the energy difference between the oscillators [8], [9] and thus has the form of thermodynamic energy flow, where the oscillator energy plays the role of temperature.

Another approach to analyzing energy flow is to focus on the return time of the energy, which characterizes the transition from reversibility to irreversibility. The analysis of this phenomenon is based on model reduction in [10] and based on a collection of oscillators with a stiffness distribution in [11]. In both cases, the transient energy flow is oscillatory and thus is not thermodynamic. An alternative approach to analyzing energy flow is to average the system energy over time [12], [13], [14]. This approach yields an equipartition result for the averaged kinetic and potential energy.

An alternative approach to modeling thermodynamic energy flow is to apply passivity theory from a control perspective [15].

The goal of the present paper is to investigate the emergence of thermodynamic energy flow without resorting to averaging, over either the external forcing, the model parameters, or time. Instead, the goal is to consider the emergence of thermodynamic energy flow as a deterministic pointwise-in-time phenomenon arising from a large number of degrees

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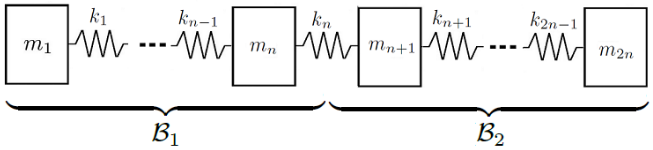


Fig. 1: Body 1 ($\mathcal{B}_1$) and Body 2 ($\mathcal{B}_2$) are comprised of coupled oscillators. $\mathcal{B}_1$ and $\mathcal{B}_2$ are connected by the spring with stiffness k_n, whose potential energy is evenly divided between $\mathcal{B}_1$ and $\mathcal{B}_2$.

of freedom. Without averaging over stochastic forcing, a stochastic model ensemble, or time, thermodynamic energy flow is viewed as a physical phenomenon arising solely due to dimension and consistent with physical observation.

To investigate this question, we consider two strings of coupled masses, where the masses are connected pairwise by springs. No dashpots are included, and thus energy is conserved. The numerical investigation shows that, for a special initial energy distribution, the energy flow between the two collections of coupled masses exhibits unidirectional energy flow, which indicates thermodynamic energy flow. As expected, the return time of the energy increases with the number of degrees of freedom, thus illustrating the transition from reversibility to irreversibility.

Beyond these expected observations, the quantitative nature of the energy flow is surprising. In particular, it turns out that the rate of energy flow is not exponential, as would be expected by the linear model (1), (2). Instead, we show that, after an initial transient and before energy return, the energy flow is more closely fit by an inverse time model than an exponential model. This characteristic is then shown to arise from a quadratically nonlinear version of Newton's law of cooling. The solution to this quadratic model is given in closed form, and estimates of the heat-transfer coefficient are given in terms of the problem data.

II. Collections of Coupled Oscillators

Consider the string of coupled oscillators shown in Figure 1, where $m_1, \ldots, m_{2n}$ are masses and $k_1, \ldots, k_{2n-1}$ are the stiffness coefficients of the springs.

The coupled oscillators shown in Figure 1 comprise two identical subsystems $\mathcal{B}_1$ and $\mathcal{B}_2$, where $\mathcal{B}_1$ consists of the masses $m_1, \ldots, m_n$ and half of the spring k_n, and $\mathcal{B}_2$ consists of the masses $m_{n+1}, \ldots, m_{2n}$ and half of the spring k_n.

Let E_1 and E_2 denote the total energy in $\mathcal{B}_1$ and $\mathcal{B}_2$, respectively, then

$$E_1 = \sum_{i=1}^{n} \frac{1}{2} m_i \dot{q}_i^2 + \sum_{i=1}^{n-1} \frac{1}{2} k_i (q_{i+1} - q_i)^2 + \frac{1}{4} k_n (q_{n+1} - q_n)^2, \tag{5}$$

$$E_2 = \sum_{i=n+1}^{2n} \frac{1}{2} m_i \dot{q}_i^2 + \sum_{i=n+1}^{2n-1} \frac{1}{2} k_i (q_{i+1} - q_i)^2 + \frac{1}{4} k_n (q_{n+1} - q_n)^2, \tag{6}$$

where for all $i = 1, \ldots, 2n$, q_i and $\dot{q}_i$ denote the displacement of m_i from its equilibrium position, and the velocity of m_i, respectively.

Consider the state space model of the system shown in Figure 1 given by

$$\dot{x} = Ax, \tag{7}$$

$$x(0) = x_0, \tag{8}$$

where $x \triangleq [q_1 \cdots q_{2n}\, \dot{q}_1 \cdots \dot{q}_{2n}]^{\mathrm{T}}$,

$$A \triangleq \begin{bmatrix} 0_{2n\times 2n} & I_{2n\times 2n} \\ -M^{-1}K & 0_{2n\times 2n} \end{bmatrix}, \tag{9}$$

$M \triangleq \operatorname{diag}(m_1, \ldots, m_{2n})$, and

$$K \triangleq \begin{bmatrix} -k_1 & k_1 & 0 & \cdots & 0 \\ k_1 & -(k_1+k_2) & k_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & k_{2n-1} & -(k_{2n-2}+k_{2n-1}) & k_{2n-1} \end{bmatrix}. \tag{10}$$

Note that the total energy of the system $E_{\text{total}} \triangleq E_1 + E_2$ is constant.

Note that (5) and (6) are functions of the squares of the the states of (7), (8). Therefore, E_1 and E_2 cannot be written as outputs of (7), (8).

Next, define $\mathcal{X} \triangleq x \otimes x$, where $\otimes$ denotes the Kronecker product. Then, using (7)

$$\begin{aligned} \dot{\mathcal{X}} &= \dot{x} \otimes x + x \otimes \dot{x} \\ &= Ax \otimes x + x \otimes Ax \\ &= (A \otimes I) x \otimes x + (I \otimes A) x \otimes x \\ &= (A \oplus A) x \otimes x \\ &= \mathcal{A}\mathcal{X}, \end{aligned} \tag{11}$$

where $\oplus$ denotes the Kronecker sum and $\mathcal{A} \triangleq A \oplus A$. Since the states of (11) are the quadratic product of the states in (7), then (5) and (6) can be written as outputs of (11) with $\mathcal{X}(0) \triangleq x(0) \otimes x(0)$. Note that (11) captures all quadratic products of the states but is nevertheless linear.

III. Energy Flow between Collections of Coupled Oscillators

Consider the initial condition $x(0) = e_{i,4n}$, where $e_{i,4n} \in \mathbb{R}^{4n}$ is the ith unit vector and $i \in \{1, \ldots, n\}$, which corresponds to moving one of the masses of $\mathcal{B}_1$ from its equilibrium position. Suppose that $n = 100$, and for all $i = 1, \ldots, n$, $m_i = 1$ kg and $k_i = 1$ N/m, then Figure 2 shows E_1, E_2, and E_{total} for different initial conditions. Note from Figure 2 that, as the mass given the nonzero initial displacement is closer to the spring connecting $\mathcal{B}_1$ and $\mathcal{B}_2$, the energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ becomes more thermodynamic. Therefore, for the remainder of the paper, we consider the initial condition $x(0) = e_{n-1,4n}$, which corresponds to assigning E_1 a nonzero initial value while the initial value of E_2 is zero. Note that the initial condition

$x(0) = e_{n,4n}$ is not chosen because this results in giving both E_1 and E_2 nonzero initial values.

Next, consider the energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ as n increases, where $x_0 = e_{n-1,4n}$, and for all $i = 1, \ldots, 2n$, $m_i = 1$ kg and for all $i = 1, \ldots, 2n-1$, $k_i = 1$ N/m. Note from Figure 3 that as n increases, the energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ remains thermodynamic over a longer time interval.

For the collections of coupled oscillators, Newton's law of cooling has the form

$$\dot{E}_1(t) = \alpha(E_2(t) - E_1(t)), \tag{12}$$

$$\dot{E}_2(t) = \alpha(E_1(t) - E_2(t)). \tag{13}$$

As shown in Section I, the solution of (12), (13) is given by

$$E_1(t) = \frac{E_1(0) - E_2(0)}{2} e^{-2\alpha t} + \frac{E_1(0) + E_2(0)}{2}, \tag{14}$$

$$E_2(t) = \frac{E_2(0) - E_1(0)}{2} e^{-2\alpha t} + \frac{E_1(0) + E_2(0)}{2}, \tag{15}$$

which exhibits exponential decay, which each energy state converging mononotically to the same equilibrium value $\frac{E_1(0)+E_2(0)}{2}$. Since the model (12), (13) is linear in the parameter α, then to obtain the value of α used in the model (12), (13), we can use least squares with samples of E_1 and E_2 obtained from simulating the system shown in Figure 1 with the initial condition $x_0 = e_{n-1,4n}$. The least squares estimate $\hat{\alpha}_{L_0,L} \in \mathbb{R}$ of α is given by

$$\hat{\alpha}_{L_0,L} \triangleq \arg\min_{\bar{\alpha}} \|\Phi_{1,L_0,L} - \bar{\alpha}\Psi_{1,L_0,L}\|_2, \tag{16}$$

where L_0 is a time step after the transient energy flow ends, and $L > L_0$ is a time step before energy reversal starts,

$$\Phi_{1,L_0,L} \triangleq \left[\begin{array}{ccc} \dot{E}_1(L_0) & \cdots & \dot{E}_1(L) \end{array} \right], \tag{17}$$

$$\Psi_{1,L_0,L} \triangleq \left[\begin{array}{ccc} E_2(L_0) - E_1(L_0) & \cdots & E_2(L) - E_1(L) \end{array} \right]. \tag{18}$$

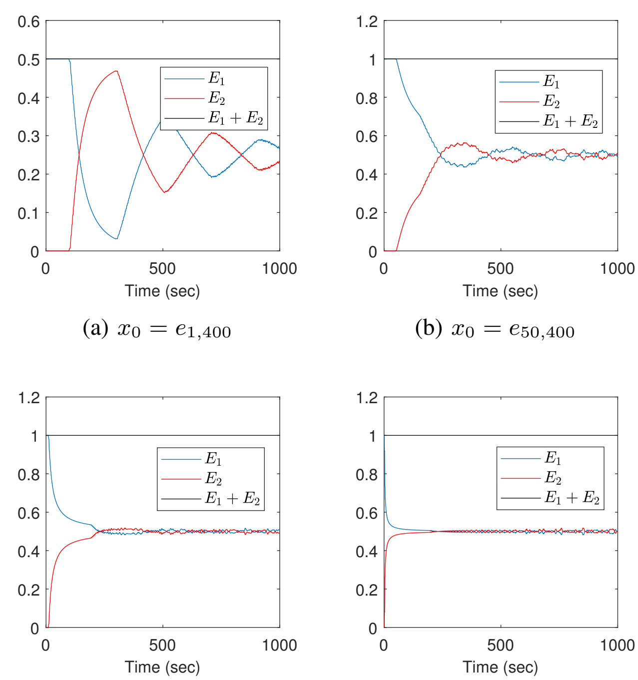
Considering the initial condition $x_0 = e_{n-1,4n}$ with $n = 200$, which corresponds to $E_1(0) = 1$ and $E_2(0) = 0$, the least squares solution obtained from (16) is $\hat{\alpha}_{L_0,L} = 0.04125$. Figure 4 shows that the model (14), (15) does not fit the simulated energy flow for the collections of coupled oscillators.

In the next section we present a modification of (12), (13) that provides a better model of the energy flow between the collections of coupled oscillators.

IV. Newton's Law of Cooling with Quadratic Dynamics

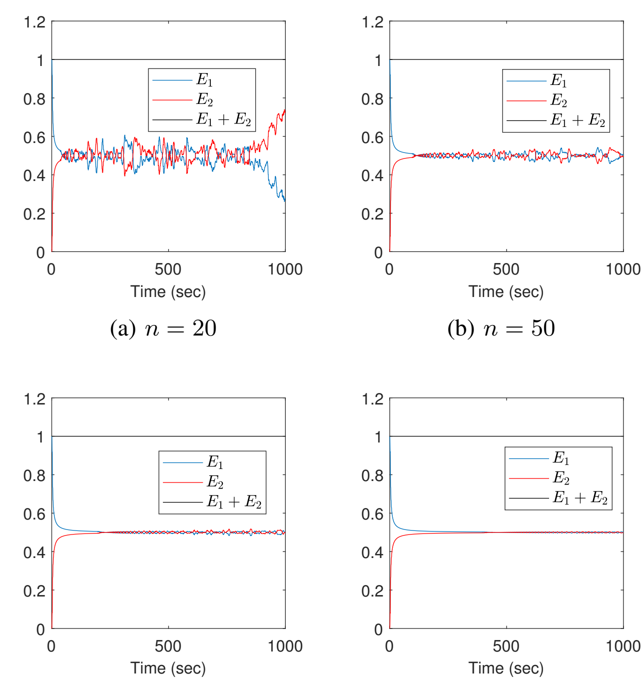
As shown in Section III, the classical version of Newton's law of cooling does not provide a satisfactory model of the energy flow between collections of coupled oscillators.

Note that the rate of energy transfer between the collections of coupled oscillators is slower than exponential. In



(a) $x_0 = e_{1,400}$ (b) $x_0 = e_{50,400}$ (c) $x_0 = e_{90,400}$ (d) $x_0 = e_{99,400}$

Fig. 2: Energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ for the initial conditions (a) $x_0 = e_{1,400}$, (b) $x_0 = e_{50,400}$, (c) $x_0 = e_{90,400}$, and (d) $x_0 = e_{99,400}$, where $n = 100$ and for all $i = 1, \ldots, 200$, $m_i = 1$ kg, and for all $i = 1, \ldots, 199$, $k_i = 1$ N/m. Note that, as the mass given the nonzero initial displacement is closer to the spring connecting $\mathcal{B}_1$ and $\mathcal{B}_2$, the energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ becomes increasingly thermodynamic.



(a) $n = 20$ (b) $n = 50$ (c) $n = 100$ (d) $n = 200$

Fig. 3: Energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ for the cases of (a) $n = 20$, (b) $n = 50$, (c) $n = 100$, and (d) $n = 200$, where $x_0 = e_{n-1,4n}$ for all cases, and for all $i = 1, \ldots, 2n$, $m_i = 1$ kg and for all $i = 1, \ldots, 2n-1$, $k_i = 1$ N/m. Note that, as n increases, the energy flow between $\mathcal{B}_1$ and $\mathcal{B}_2$ remains thermodynamic over a longer time interval.

particular, it can be seen that the energy of Body 2 is zero at $t = 0$ and is close to $\frac{1}{2}E_{\rm total}$ before energy return begins. This suggests a viable expression for the energy of Body 2 of the form $t/(2t + a)$. Figure 5 compares this expression to the computed energy of Body 2 with $a = 4$. Note that, after the initial transient and over a finite interval, namely, before energy return begins, the expression $t/(2t+a)$ closely approximates the computed energy of Body 2.

Next, to obtain a suitable thermodynamic energy-flow model consider the quadratic model

$$\dot{E}_1(t) = \beta_1 E_1(t)^2 + \beta_2 E_2(t)^2 + \beta_3 E_1(t)E_2(t), \quad (19)$$
$$\dot{E}_2(t) = -\dot{E}_1(t), \quad (20)$$

where β_1, β_2, and β_3 are constants. Since the model (19), (20) is linear in the parameters, we can use least squares with samples of E_1 and E_2 obtained from simulating the system shown in Figure 1 with the initial condition $x_0 = e_{n-1,4n}$ to estimate β_1, β_2, and β_3. The least squares estimate is given by

$$\hat{\theta}_{L_0,L} \triangleq \arg\min_{\bar{\theta}} \|\Phi_{2,L_0,L} - \bar{\theta}\Psi_{2,L_0,L}\|_2, \quad (21)$$

where $\hat{\theta}_{L_0,L} \in \mathbb{R}^{1\times 3}$ is an estimate of $\theta \triangleq [\beta_1\ \beta_2\ \beta_3]$, L_0 is a time step after the transient energy flow ends, and $L > L_0$ is a time step before energy reversal starts,

$$\Phi_{2,L_0,L} \triangleq \left[\ \dot{E}_1(L_0) \quad \cdots \quad \dot{E}_1(L)\ \right], \quad (22)$$
$$\Psi_{2,L_0,L} \triangleq \begin{bmatrix} E_1(L_0)^2 & \cdots & E_1(L)^2 \\ E_2(L_0)^2 & \cdots & E_2(L)^2 \\ E_1(L_0)E_2(L_0) & \cdots & E_1(L)E_2(L) \end{bmatrix}. \quad (23)$$

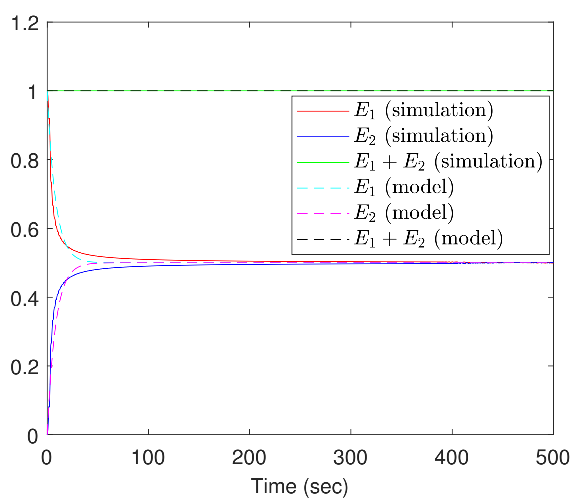


Fig. 4: E_1 and E_2 obtained from simulating the system shown in Figure 1 with $n = 200$ and the initial condition $x_0 = e_{n-1,4n}$, and the solutions (14) and (15) obtained with $\alpha = 0.04125$, $E_1(0) = 1$ and $E_2(0) = 0$. This plot suggests that the linear model (12), (13) of the energy flow between Body 1 and Body 2 is not accurate.

Considering the initial condition $x_0 = e_{n-1,4n}$ with $n = 200$, which corresponds to $E_1(0) = 1$ and $E_2(0) = 0$, the least squares solution obtained from (21) is $\hat{\theta}_{L_0,L} = 0.25[1\ 1\ -2]$, that is, $\beta_1 = \beta_2 = -\frac{1}{2}\beta_3$.

Based on the least squares solution, we consider a variation of Newton's law of cooling given by the quadratic dynamics

$$\dot{E}_1(t) = \alpha \mathrm{sign}(E_2(t) - E_1(t))(E_2(t) - E_1(t))^2, \quad (24)$$
$$\dot{E}_2(t) = \alpha \mathrm{sign}(E_1(t) - E_2(t))(E_2(t) - E_1(t))^2. \quad (25)$$

Note that (24), (25) is a quadratically nonlinear compartmental model for thermodynamic energy flow. The solution of (24), (25) is given by

$$E_1(t) = \frac{\alpha \mathrm{sign}(E_2(t) - E_1(t))(E_2(0)^2 - E_1(0)^2)t + E_1(0)}{2\alpha \mathrm{sign}(E_2(t) - E_1(t))(E_2(0) - E_1(0))t + 1}, \quad (26)$$

$$E_2(t) = \frac{\alpha \mathrm{sign}(E_2(t) - E_1(t))(E_2(0)^2 - E_1(0)^2)t + E_2(0)}{2\alpha \mathrm{sign}(E_2(t) - E_1(t))(E_2(0) - E_1(0))t + 1}. \quad (27)$$

Note that, as in the case of Newton's law of cooling (14), (15), the states E_1 and E_2 of (26), (27) converge monotonically to the equilibrium energy $\frac{E_1(0)+E_2(0)}{2}$. However, instead of exponential convergence as in (14), (15) due to linear dynamics, the convergence in (26), (27) is asymptotic but not exponential due to the quadratically nonlinear dynamics of (24), (25).

Figure 5 shows a plot of E_1 and E_2 obtained from simulating the system shown in Figure 1 with $n = 200$ and the initial condition $x_0 = e_{n-1,4n}$, and the solutions (26) and (27) obtained with $\alpha = 0.25$, $E_1(0) = 1$ and $E_2(0) = 0$. Figure 5 suggests that the quadratic model (19), (20) of the energy flow between Body 1 and Body 2 is more accurate than the linear model (12), (2) whose energy flow is shown in Figure 4.

V. Conclusions

This paper investigated thermodynamic energy flow as an emergent phenomenon. The goal was to demonstrate thermodynamic energy flow without averaging over inputs, model parameters, or time. Unlike stochastically or temporally averaged responses, deterministic, pointwise-in-time thermodynamic energy flow reflects the physically observed laws of thermodynamics.

Deterministic, pointwise-in-time thermodynamic energy flow was demonstrated in this paper for collections of coupled oscillators. Surprisingly, the rate of energy flow was found to be inconsistent with the classical exponential response corresponding to Newton's law of cooling, whose dynamics are linear. Instead, the rate of energy flow was shown to be consistent with the response of a thermodynamic energy-flow model with quadratically nonlinear dynamics. The primary goal of future research is to demonstrate this behavior as an asymptotic property of the system dimension.

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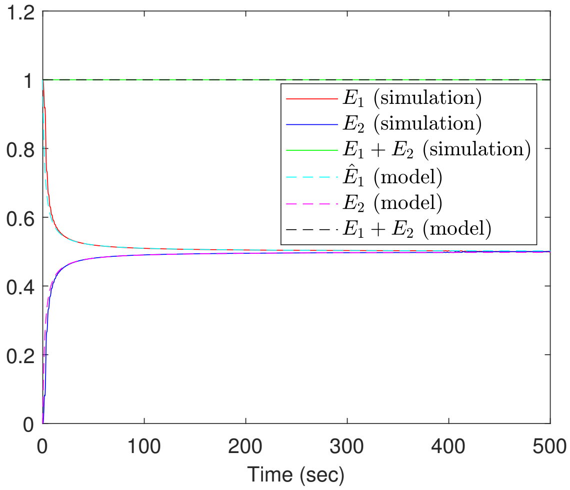

Fig. 5: E_1 and E_2 obtained from simulating the system shown in Figure 1 with $n = 200$ and the initial condition $x_0 = e_{n-1,4n}$, and the solutions (26) and (27) obtained with $\alpha = 0.25$, $E_1(0) = 1$ and $E_2(0) = 0$. This plot shows that the quadratically nonlinear energy-flow model (19), (20) for the energy flow between Body 1 and Body 2 is much more accurate than the linear energy-flow model (12), (13), whose solution is shown in Figure 4.

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