Entropy and Energy Measures: Complementary Tools for Analyzing Reaction Diffusion Dynamics

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Introduction

- Tools from **statistical mechanics** (entropy) and **physics** (energy norm) provide insights into **phase transitions and emergent behavior** of systems [8].
- **Reaction-diffusion** systems exhibit behavior akin to classical thermodynamic systems [4].
- **Goal**: Apply and **compare** the of tools **entropy** and **energy** to characterize reaction-diffusion system behavior.

Background

Reaction-Diffusion Systems:

- Exhibit rich pattern formation and phase transitions.
- Coupled equations model processes involving competing forces of reaction and diffusion.
- Examples: *biological patterns*, *chemical instabilities* [6]

Entropy Measure: Shown to quantify global uncertainty and phase boundaries [5].

Energy Norm: Captures both global deviations and localized oscillatory behavior [3, 7, 9].

Mathematical Problem Setup

Schnakenberg model [10]:

$$\frac{\partial u_1}{\partial t} = D_1 \Delta u_1 - R_1(u_1, u_2) u_1 + K_1 \qquad \text{on } \Omega \times [0, t_{end}],$$
$$\frac{\partial u_2}{\partial t} = D_2 \Delta u_2 - R_2(u_1, u_2) u_2 + K_2 \qquad \text{on } \Omega \times [0, t_{end}],$$

$$R_1(u_1, u_2) = \gamma - \gamma u_1 u_2,$$
$$R_2(u_1, u_2) = \gamma u_1^2,$$
$$K_1 = \gamma a,$$
$$K_2 = \gamma b.$$

Mathematical Problem Setup

Parameterize:

- Define **diffusion ratio** $d = D_2/D_1$
- Define **reactivity** γ
- Fix a, b according to [1]
- Problem defined solely by $(\gamma, d) \in \mathcal{P}$

Initial Conditions:

- Perturbations (ε) from steady state of u_1 [2]:

$$u_{1,ss} + \varepsilon = (a + b) + \varepsilon,$$

$$u_{2,ss} = \frac{b}{(a + b)^2}.$$

Numerical Solution Scheme

Finite Element Method and Implicit Euler:

$$a(u,v) = \langle u, v\rangle + h_t d \langle \nabla u, \nabla v\rangle + h_t \langle R(u_{prev})u, v\rangle\,, \tag{1}$$
$$l(v) = \langle u_{prev} + K, v\rangle\,. \tag{2}$$

Linear System:

$$\mathbf{u}^{(n+1)} = (M + D + R^{(n)})^{-1}\mathbf{f}^{(n)}$$

Mesh:

- Linear triangular basis functions
- 50 nodes on $\Omega_h = [0,3]\times[0,3]$, $h_t = 0.01$, and $t_{end} = 0.3$

Methods

Entropy Measure:

$$S(u_t) = |s(u_t) - s(u_{ss})|, \quad s(x) = -\sum \hat{x}_{i,j} \log \hat{x}_{i,j}.$$

Energy Norm:

$$E(u_t) = |\|u_t\|_E - \|u_{ss}\|_E, \quad \|u\|_E = \|\nabla u\|_2 + \|u\|_2.$$

Experiment: Solve problem for array of $(\gamma, d) \in \mathcal{P}$

- Examine only u_1 since u_2 is similar but out of phase

Results: Time Domain Analysis

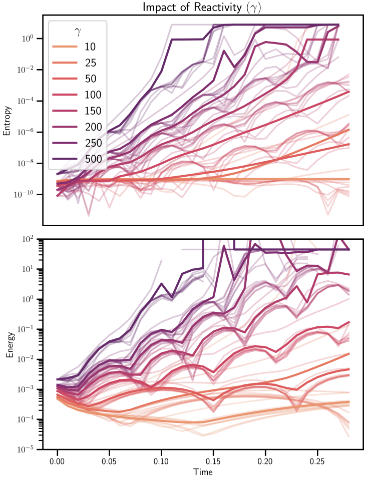

Figure 1. Time domain analysis of entropy and energy measures over time, revealing the impact of γ.

Rate of deviation from SS increases with γ

- **Entropy**
  - Exponential growth
  - Variation within γ
- **Energy**
  - Nonlinearity
  - Clearer grouping by γ

Results: Frequency Domain Analysis

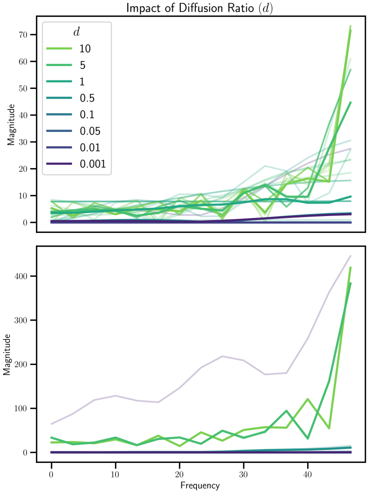

Figure 2. Spectrum of entropy and energy measures over time revealing the impact of d.

Increasing d amplifies spectrum, particularly higher frequencies

- **Entropy**
  - Gradual transition with d
  - Variation within d
- **Energy**
  - Sharp jump in magnitude
  - Clearer grouping by d

Results: Phase Plots and System Behavior

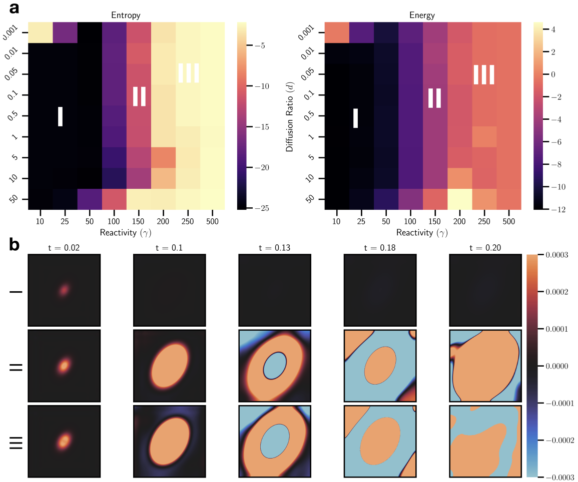

Figure 3. **(a)** Heatmap phase plots of the integrated energy and entropy measures for points $(\gamma, d) \in \mathcal{P}$. **(b)** Numerical solutions of the reaction diffusion system for three representative points in the parameter space.

Discussion

- **Entropy:** Smooth trends in time and frequency domain and detects phase boundaries when integrated.
- **Energy:** Separates effects of γ and d, while revealing finer detail of behavior when integrated.
- **Future Work:**
  - Improve phase plot measure to show impact of d, add more time points or incorporate frequency domain.
  - Higher order basis functions to enforce boundary conditions.
  - Compare with other characterization techniques such bifurcation analysis.
- **Applications**:
  - Detection of phase shifts for control using entropy.
  - Parameter estimation of dynamical systems using energy.

Conclusion

Entropy and energy measures provide **complementary tools**, together providing detailed insights into system behavior.

The results demonstrate the effectiveness of **borrowing tools** from other disciplines.

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Thank You

Questions?