A Note on Algorithmic Behavior in Molecular Systems

(Preliminary Definitions and Scope)

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1. Motivation

Biological systems exhibit reproducible, goal-directed behaviors across molecular, cellular, and tissue scales, despite operating in regimes where individual microscopic trajectories are fundamentally stochastic and unpredictable. Yet these systems reliably implement conditional responses, sequential actions, and context-dependent outcomes.

This note addresses how such behaviors can be **explained without requiring** symbolic computation, digital determinism, or exact trajectory predictability at the molecular level.

The purpose of this work is not to present a complete formal theory, but to establish a **minimal, physically grounded definition of algorithmic and logical behavior in molecular systems**, grounded in energy, state accessibility, probability flow, and interaction constraints.

Crucially, this work adopts the position that **logic is not imposed on biological systems as an abstract rule set, but enacted by them through physical constraint**.

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2. System Description

We consider a biological system as an **open, driven, stochastic dynamical system** composed of interacting molecular agents embedded in a structured cellular environment.

Definition 1 (Molecular Agent)

A molecular agent is any molecular entity (e.g., RNA, protein, molecular complex, or assembly) characterized by:

- a finite set of internal states (e.g., conformations, binding states, chemical states),
- spatial degrees of freedom within a cellular environment,
- interaction rules governed by physical laws, including diffusion, sterics, electrostatics, and chemical kinetics.

Molecular agents do not execute symbolic instructions; instead, they **select among physically accessible futures through conditional interactions**.

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3. State and Dynamics

Definition 2 (System State)

The state of the system at time t is defined as a **probability distribution over accessible microstates**:

$$\mathcal{S}(t) = \{P(x_i, E_i, r_i, \ldots)\}$$

where each microstate x_i represents a specific configuration of agents, associated with energy E_i, spatial coordinates r_i, and interaction context.

Exact trajectories of individual microstates are **not assumed to be predictable or reproducible**.

Definition 3 (Transition Dynamics)

State evolution is governed by **stochastic transitions**:

$$P(s_i \to s_j) = K_{ij}(\Theta)$$

where the transition kernel K_{ij} depends on:

- encounter probability (diffusion, localization, copy number, lifetime),
- thermodynamic selectivity (free-energy differences, activation barriers),
- environmental parameters Θ (temperature, crowding, compartmentalization).

These kernels define which transitions are **enabled, suppressed, or conditionally accessible**.

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4. Emergence of Algorithmic Behavior

Definition 4 (Algorithmic Molecular Network)

An algorithmic molecular network is a molecular interaction network whose structure **imposes conditional constraints on state transitions** such that, over time, **probability mass is systematically biased toward a restricted subset of macroscopic outcomes**.

Algorithmic behavior does not imply symbolic logic or discrete instruction execution. Instead, it refers to:

- constrained probability flow,
- reproducible ensemble-level outcomes,
- conditional dependence of accessible futures on prior system states and interactions.

In this framework, **emergence is not arbitrary pattern formation**, but the manifestation of **conditional constraints that enforce reproducible decision structure**.

Definition 5 (Logical Operation)

A logical operation is defined as a **reproducible, condition-dependent redistribution of probability mass over system states**, enacted through physical interaction constraints.

Examples include:

- **Activation**: probability shifts toward states enabling downstream reactions.
- **Inhibition**: probability is redirected away from a pathway or basin of attraction.
- **AND-like behavior**: a transition requires multiple rare encounters within a bounded temporal or spatial window.
- **NOT-like behavior**: one interaction suppresses or diverts probability flow initiated by another.

These operations constitute **logic implemented physically, not symbolically**: they realize conditional branching and exclusion at the ensemble level.

Deterministic Execution and Probabilistic Access

Logical operations at the molecular level are **executed deterministically upon interaction**: when the required molecular agents encounter each other under appropriate physical conditions, the corresponding state transition (e.g., binding, cleavage, activation) occurs with high reliability. However, whether such interactions occur within a given time interval is governed by **stochastic access processes**, including diffusion, spatial localization, copy number, molecular lifetime, and compartmentalization.

As a result, molecular logic is **not probabilistic in execution but probabilistic in access**: deterministic local rules are activated on a stochastic schedule, and the probability of state transformation over a finite time window is determined by encounter statistics rather than partial or graded reaction outcomes.

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5. Predictability and Scale

Exact prediction of microscopic trajectories is generally impossible due to:

- high dimensionality,
- stochastic encounters,
- non-integrability of interacting many-body systems.

However, **ensemble-level trends, steady states, and conditional probabilities are predictable**, analogous to:

- statistical mechanics,
- reaction–diffusion systems,
- weather and climate models.

Algorithmic and logical behavior is therefore defined at the level of **probability distributions and accessibility constraints**, not at the level of individual molecular events.

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6. Multiscale Propagation

Algorithmic constraints can propagate across scales through **coarse-graining**:

- **Molecular scale**: interaction energies, diffusion, binding specificity.
- **Cellular scale**: regulatory networks, compartmentalization, feedback loops.
- **Tissue scale**: cell–cell signaling, geometry, gradients.

While microstate detail is lost at higher scales, **constraint structure is preserved**, enabling stable, reproducible macroscopic behavior.

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7. Scope and Limitations

This note does **not** claim:

- digital or symbolic computation in biology,
- exact controllability of molecular systems,
- closed-form predictability of biological dynamics.

Instead, it provides a **physically grounded framework** in which logic and algorithmic behavior arise as **material properties of constrained stochastic systems**.

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8. Outlook

A full formalism would require:

- explicit construction of state spaces,
- quantitative encounter and lifetime models,
- thermodynamic and kinetic parameterization,
- compositional rules for modular molecular systems.

These developments are deferred to future work, including **direct application of the present definitions to logical biomolecular complexes (LBCs), RNA toehold systems, and viral program architectures**.