

Deterministic Symbiosis and Finite-Time Molecular Self-Regulation: A Closed-Form Dynamical Framework for Macromolecular Equilibrium and Distance Geometry

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Abstract

Context: Macromolecular structure prediction and conformational energy relaxation have historically relied on stochastic heuristics, Monte Carlo sampling, and deep statistical neural networks (e.g., AlphaFold), which are stochastic or statistical in formulation and can have non-zero predictive uncertainty, with computational costs that depend strongly on the method and implementation. **Objective:** This work introduces the *Deterministic Symbiosis Engine*, a closed-form, finite-state feedback operator designed for autonomous energetic equilibrium, mass convergence, and Euclidean distance geometry resolution without stochastic variables or black-box heuristics. **Method:** The state operator $\mathcal{T} : (E, M) \mapsto (E', M')$ acts as a non-linear piecewise dead-band contractor over a designated energy interval $\mathcal{I}_{\text{symb}} = [E_{\text{opt}} - \epsilon, E_{\text{opt}} + \epsilon]$. We generalize $\mathcal{T}$ into an N -dimensional tensorial map incorporating angular momentum tensors $\mathbf{J}$ and local hydrodynamic dissipation matrices $\mathbf{\Gamma}$. **Results:** We prove that for $2\epsilon \geq \max(\Delta E_{\text{inc}}, \Delta E_{\text{dec}})$, limit cycles are strictly precluded, yielding exact closed-form convergence in K_i steps. For a benchmark suite of 7 heterogeneous molecular subunits, the maximum individual convergence horizon is $K_{\text{total}} = 4$ under the stated parameters, with $\Delta_{\text{dev}} = 0$ in the fixed implementation. The perturbation test returns to the dead-band in $K_{\text{pert}} = 2$ cycles under the stated benchmark conditions. **Conclusion:** By embedding $\mathcal{T}$ within Euclidean Distance Matrix (EDM) completion via semidefinite algebraic constraints, this framework demonstrates $O(N)$ computational complexity for uncoupled systems and a conditional Lyapunov analysis for the coupled consensus dynamics, establishing a deterministic foundation for computational structural biophysics.

Keywords: Deterministic Dynamics, Finite-Time Convergence, Dead-Band Control, Lyapunov Stability, Distance Geometry, Macromolecular Folding.

1 Introduction

The determination of macromolecular tertiary structure and thermodynamic relaxation remains one of the foundational challenges in biophysics. For decades, the dominant paradigms have encompassed Molecular Dynamics

(MD) numerical integration [2], Markov Chain Monte Carlo (MCMC) simulations [3], and deep generative networks [1]. While empirical predictive accuracy has expanded substantially through overparameterized neural architectures, these methods operate as probabilistic or heuristic approximations possessing intrinsic stochastic fluctuations and high algorithmic complexity ($O(N^2)$ to $O(N^3)$ per sweep).

In contrast, biological self-organization operates within strictly bounded physical tolerances governed by localized feedback mechanisms, mass transfer gradients, and stereochemical invariance. This paper formulates the *Deterministic Symbiosis and Molecular Self-Regulation Engine*, an analytical finite-state feedback system. The engine operates deterministically:

- (i) It eliminates pseudo-random seeds and probabilistic sampling, ensuring exact reproducibility ($\Delta_{\text{dev}} = 0$).
- (ii) It establishes an analytic closed-form expression for the discrete relaxation time K_i .
- (iii) It enforces strict stability via piecewise dissipative energy-mass maps over phase-space attractors.

The document is organized as follows: Section 2 defines the fundamental 2D state space, operator $\mathcal{T}$, and convergence results. Section 3 reports the benchmark suite of 7 subunits and analyzes phase-space trajectories under perturbation. Section 4 presents the N -dimensional tensorial generalization incorporating angular momentum and hydrodynamic damping. Section 5 derives the computational complexity scaling. Section 6 gives a conditional Lyapunov analysis of the coupled consensus dynamics. Finally, Section 7 formulates the Euclidean Distance Matrix (EDM) reconstruction problem.

2 Mathematical Formulation and State Operator

2.1 State Vector and Symbiotic Target Set

Let $\mathcal{S} = \{e_1, e_2, \dots, e_N\}$ denote an ensemble of N interacting molecular subunits. The state of subunit e_i at

discrete cycle $k \in \mathbb{N}_0$ is parameterized by the vector:

$$\mathbf{x}_i^{(k)} = \begin{pmatrix} E_i^{(k)} \\ M_i^{(k)} \end{pmatrix} \in \mathbb{R}^2, \quad (1)$$

where $E_i^{(k)} \in \mathbb{R}$ represents the effective conformational energy (in arbitrary computational units or kcal/mol) and $M_i^{(k)} \in \mathbb{R}^+$ denotes the effective subunit mass (in Daltons, Da).

Definition 1 (Symbiosis Window / Decoupled Invariant Set). *Given an optimal baseline energy $E_{\text{opt}} \in \mathbb{R}$ and a half-tolerance bandwidth $\epsilon > 0$, the Symbiosis Target Interval $\mathcal{I}_{\text{symb}}$ is defined as the compact subset:*

$$\mathcal{I}_{\text{symb}} = [E_{\text{opt}} - \epsilon, E_{\text{opt}} + \epsilon] \subset \mathbb{R}. \quad (2)$$

For the uncoupled operator $\mathcal{T}$, the corresponding fixed set in the (E, M) phase space is the cylinder $\mathcal{A}_{\text{symb}} = \mathcal{I}_{\text{symb}} \times \mathbb{R}^+$. This invariance statement applies to the decoupled operator; additional coupling terms require separate conditions.

2.2 Piecewise Discrete Transformation Operator

The evolution of state $\mathbf{x}_i^{(k)}$ across discrete cycles $k \rightarrow k+1$ is governed by the nonlinear mapping $\mathcal{T} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$:

$$\mathbf{x}_i^{(k+1)} = \mathcal{T}(\mathbf{x}_i^{(k)}) = \begin{pmatrix} E_i^{(k)} + u(E_i^{(k)}) \\ M_i^{(k)} + v(E_i^{(k)}) \end{pmatrix}, \quad (3)$$

where the energetic controller $u(E)$ and the mass transfer controller $v(E)$ are piecewise constant functions:

$$u(E) = \begin{cases} +\Delta E_{\text{inc}}, & \text{if } E < E_{\text{opt}} - \epsilon \quad (\text{accumulation}), \\ -\Delta E_{\text{dec}}, & \text{if } E > E_{\text{opt}} + \epsilon \quad (\text{dissipation}), \\ 0, & \text{if } E \in \mathcal{I}_{\text{symb}} \quad (\text{active symbiosis}), \end{cases} \quad (4)$$

$$v(E) = \begin{cases} +\Delta M_{\text{inc}}, & \text{if } E < E_{\text{opt}} - \epsilon, \\ -\Delta M_{\text{dec}}, & \text{if } E > E_{\text{opt}} + \epsilon, \\ 0, & \text{if } E \in \mathcal{I}_{\text{symb}}. \end{cases} \quad (5)$$

The nominal calibration parameters investigated herein are:

$$\begin{aligned} E_{\text{opt}} &= 500.0, & \epsilon &= 50.0 \implies \mathcal{I}_{\text{symb}} = [450.0, 550.0], \\ \Delta E_{\text{inc}} &= 70.0, & \Delta M_{\text{inc}} &= 5.0 \text{ Da}, \\ \Delta E_{\text{dec}} &= 90.0, & \Delta M_{\text{dec}} &= 12.0 \text{ Da}. \end{aligned} \quad (6)$$

2.3 Finite-Time Convergence and Non-Oscillation Theorems

A critical requirement for deterministic stability is the absence of boundary overshoot that could induce limit-cycle periodic orbits across $\mathcal{I}_{\text{symb}}$.

Theorem 1 (Non-Existence of Limit Cycles). *Let $\Delta E_{\text{inc}} > 0$ and $\Delta E_{\text{dec}} > 0$. If the bandwidth of the symbiotic attractor satisfies:*

$$2\epsilon \geq \max(\Delta E_{\text{inc}}, \Delta E_{\text{dec}}), \quad (7)$$

then every trajectory of the uncoupled energy map reaches $\mathcal{I}_{\text{symb}}$ in finite time and remains there. Consequently, the map has no periodic orbit of period $p \geq 2$.

Proof. Consider an initial energy in the accumulation zone $E^{(0)} < E_{\text{opt}} - \epsilon$. Let k^* be the smallest integer such that $E^{(k^*)} \geq E_{\text{opt}} - \epsilon$. Prior to crossing, $E^{(k^*-1)} < E_{\text{opt}} - \epsilon$. Applying the operator:

$$E^{(k^*)} = E^{(k^*-1)} + \Delta E_{\text{inc}} < E_{\text{opt}} - \epsilon + \Delta E_{\text{inc}}. \quad (8)$$

To prevent an immediate overshoot into the dissipation zone ($E > E_{\text{opt}} + \epsilon$), we require:

$$E_{\text{opt}} - \epsilon + \Delta E_{\text{inc}} \leq E_{\text{opt}} + \epsilon \iff \Delta E_{\text{inc}} \leq 2\epsilon. \quad (9)$$

Similarly, for a state initialized in the dissipation zone $E^{(0)} > E_{\text{opt}} + \epsilon$, the first cycle m^* entering $E \leq E_{\text{opt}} + \epsilon$ satisfies:

$$E^{(m^*)} = E^{(m^*-1)} - \Delta E_{\text{dec}} > E_{\text{opt}} + \epsilon - \Delta E_{\text{dec}}. \quad (10)$$

To avoid overshooting into the accumulation zone ($E < E_{\text{opt}} - \epsilon$), we require:

$$E_{\text{opt}} + \epsilon - \Delta E_{\text{dec}} \geq E_{\text{opt}} - \epsilon \iff \Delta E_{\text{dec}} \leq 2\epsilon. \quad (11)$$

Combining both inequalities yields condition (7). Since $2\epsilon = 100.0$ and $\max(70.0, 90.0) = 90.0 \leq 100.0$, the first transition from either exterior region cannot land beyond the opposite boundary. The trajectory therefore enters $\mathcal{I}_{\text{symb}}$ in finite time and remains fixed because $u(E) = 0$ for all $E \in \mathcal{I}_{\text{symb}}$. $\square$

Theorem 2 (Closed-Form Convergence Index K_i). *For any decoupled subunit e_i initialized at $\mathbf{x}_i^{(0)} = (E_i^{(0)}, M_i^{(0)})^T$ with $M_i^{(0)} > 0$ and, when $E_i^{(0)} > E_{\text{opt}} + \epsilon$, $M_i^{(0)} - K_i \Delta M_{\text{dec}} > 0$, the exact number of iterations $K_i \in \mathbb{N}_0$ required to reach active symbiosis is:*

$$K_i = \begin{cases} \left\lceil \frac{(E_{\text{opt}} - \epsilon) - E_i^{(0)}}{\Delta E_{\text{inc}}} \right\rceil, & E_i^{(0)} < E_{\text{opt}} - \epsilon, \\ \left\lceil \frac{E_i^{(0)} - (E_{\text{opt}} + \epsilon)}{\Delta E_{\text{dec}}} \right\rceil, & E_i^{(0)} > E_{\text{opt}} + \epsilon, \\ 0, & E_i^{(0)} \in \mathcal{I}_{\text{symb}}. \end{cases} \quad (12)$$

For $E_i^{(0)} \notin \mathcal{I}_{\text{symb}}$, the terminal state $\mathbf{x}_i^{(\infty)} = \mathbf{x}_i^{(K_i)}$ is evaluated in closed form as:

$$\begin{aligned} E_i^{(K_i)} &= E_i^{(0)} + K_i \cdot \text{sgn}(E_{\text{opt}} - E_i^{(0)}) \cdot \Delta E_{\star}, \\ M_i^{(K_i)} &= M_i^{(0)} + K_i \cdot \text{sgn}(E_{\text{opt}} - E_i^{(0)}) \cdot \Delta M_{\star}, \end{aligned} \quad (13)$$

where $\star \in \{\text{inc}, \text{dec}\}$ is selected according to the initial regime. If $E_i^{(0)} \in \mathcal{I}_{\text{symb}}$, then $K_i = 0$ and $\mathbf{x}_i^{(\infty)} = \mathbf{x}_i^{(0)}$.

Proof. In the linear regime $E_i^{(k)} < E_{\text{opt}} - \epsilon$, the sequence follows an arithmetic progression $E_i^{(k)} = E_i^{(0)} + k\Delta E_{\text{inc}}$. The threshold condition $E_i^{(k)} \geq E_{\text{opt}} - \epsilon$ requires $k\Delta E_{\text{inc}} \geq (E_{\text{opt}} - \epsilon) - E_i^{(0)}$. Division by $\Delta E_{\text{inc}} > 0$ and ceiling quantization yields (12). An identical argument applies to the dissipation regime. $\square$

The global convergence horizon for an uncoupled ensemble $\mathcal{S}$ is:

$$K_{\text{total}} = \max_{i \in \{1, \dots, N\}} K_i. \quad (14)$$

3 Benchmark Validation and Dynamic Stress Analysis

3.1 Deterministic Benchmark Suite

We apply operator $\mathcal{T}$ to a heterogeneous seven-element benchmark suite $\mathcal{S}_7 = \{M_1, \dots, M_7\}$. Table 1 summarizes the exact analytical trajectories and terminal states.

The global convergence horizon for the uncoupled benchmark is rigorously given by:

$$K_{\text{total}} = \max(3, 4, 0, 3, 4, 0, 0) = 4. \quad (15)$$

Thus K_{total} denotes the maximum individual convergence horizon, not the sum of all per-subunit updates. For this benchmark, $\sum_i K_i = 14$. The quantity K_{total} is therefore a completion horizon for the uncoupled ensemble. All benchmark trajectories are deterministic under the stated arithmetic implementation; the reported $\Delta_{\text{dev}} = 0$ denotes identical benchmark outputs under that fixed implementation, not a universal bitwise guarantee across all IEEE 754 hardware and compiler configurations.

3.2 Phase-Space Geometry

The (E, M) phase portrait decomposes into three parallel affine vector fields:

$$\vec{v}(E, M) = \begin{cases} (+70.0, +5.0)^T, & E < 450.0, \\ (-90.0, -12.0)^T, & E > 550.0, \\ (0.0, 0.0)^T, & E \in [450.0, 550.0]. \end{cases} \quad (16)$$

Trajectories represent piecewise straight lines in $\mathbb{R}^2$ with directional slopes:

$$\sigma_{\text{inc}} = \frac{\Delta M_{\text{inc}}}{\Delta E_{\text{inc}}} = \frac{5}{70} \approx 0.0714 \text{ Da/unit}, \quad (17)$$

$$\sigma_{\text{dec}} = \frac{\Delta M_{\text{dec}}}{\Delta E_{\text{dec}}} = \frac{12}{90} \approx 0.1333 \text{ Da/unit}. \quad (18)$$

Because the vector field vanishes on $\mathcal{A}_{\text{symb}}$, any orbit terminating in $\mathcal{A}_{\text{symb}}$ is invariant for all $k \geq K_i$.

3.3 Dynamic Perturbation and Resilience Analysis

To evaluate resilience against non-equilibrium shocks, we subject the stabilized node M_3 (initially in equilibrium at $\mathbf{x}_3 = (500.0, 130.0)$) to an instantaneous thermal impulse:

$$\delta E = +200.0 \implies \mathbf{x}_{3,\text{pert}}^{(0)} = (700.0, 130.0 \text{ Da})^T. \quad (19)$$

The perturbed node enters the thermal dissipation regime ($700.0 > 550.0$). The analytical relaxation index is:

$$K_{\text{pert}} = \left\lceil \frac{700.0 - 550.0}{90.0} \right\rceil = \left\lceil \frac{150.0}{90.0} \right\rceil = \lceil 1.6667 \rceil = 2. \quad (20)$$

The deterministic discrete trajectory unfolds as follows:

$$k = 0 : \mathbf{x}_3^{(0)} = (700.0, 130.0 \text{ Da})^T, \quad (21)$$

$$k = 1 : \mathbf{x}_3^{(1)} = (610.0, 118.0 \text{ Da})^T, \quad (22)$$

$$(700.0 - 90.0, 130.0 - 12.0)^T, \quad (23)$$

$$k = 2 : \mathbf{x}_3^{(2)} = (520.0, 106.0 \text{ Da})^T, \quad (24)$$

$$(610.0 - 90.0, 118.0 - 12.0)^T. \quad (25)$$

Because $520.0 \in [450.0, 550.0]$, the subunit re-enters active symbiosis at $k = 2$, demonstrating immediate self-healing without propagating numerical instability.

4 Tensorial N-Dimensional Extension

To model macromolecules in viscous intracellular media, the state space must encompass rotational degrees of freedom and hydrodynamic coupling.

4.1 Extended State Tensor

Let the augmented state of subunit e_i be represented by the tensor tuple:

$$\mathbf{Z}_i^{(k)} = (E_i^{(k)}, M_i^{(k)}, \mathbf{J}_i^{(k)}, \mathbf{q}_i^{(k)}) \in \mathcal{H}, \quad (26)$$

where:

- $E_i \in \mathbb{R}$ is the conformational potential energy;
- $M_i \in \mathbb{R}^+$ is the effective mass;
- $\mathbf{J}_i \in \mathbb{R}^3$ is the rotational angular momentum vector ($\mathbf{J}_i = \mathbf{I}_i \boldsymbol{\omega}_i$, with inertia tensor $\mathbf{I}_i \in \mathbb{R}^{3 \times 3}$);
- $\boldsymbol{\Gamma}_i \in \mathbb{R}^{3 \times 3}$ is the prescribed anisotropic hydrodynamic drag tensor; for a spherical approximation it reduces to $\boldsymbol{\Gamma}_i = 6\pi\eta_{\text{med}} R_i \mathbf{I}$, while a nonspherical tensor requires a separately specified hydrodynamic model;
- $\mathbf{q}_i \in \mathbb{R}^3$ is the centroid position in $\mathbb{R}^3$.

4.2 Coupled Tensorial Transformation Operator

The continuous-time hydrodynamic torque balance with deterministic discrete feedback yields the tensorial map:

$$\mathbf{Z}_i^{(k+1)} = \mathbf{Z}_i^{(k)} + \boldsymbol{\Psi}(\mathbf{Z}_i^{(k)}) + \sum_{j \neq i}^N \boldsymbol{\Omega}_{ij}(\mathbf{Z}_i^{(k)}, \mathbf{Z}_j^{(k)}), \quad (27)$$

Table 1: Deterministic Trajectory and Convergence Benchmark for 7 Molecular Subunits under Operator $\mathcal{T}$.

Subunit ID	$\mathbf{x}_i^{(0)} = (E_0, M_0)$	Operational Regime	Calculated K_i	Entrance Cycle	$\mathbf{x}_i^{(\text{final})} = (E_{\text{final}}, M_{\text{final}})$	Δ_{dev}
M_1	(300.0, 75.0 Da)	Accumulation / Resonance	$\lceil (450 - 300)/70 \rceil = 3$	Cycle 3	(510.0, 90.0 Da)	0.000
M_2	(850.0, 180.0 Da)	Thermal Dissipation	$\lceil (850 - 550)/90 \rceil = 4$	Cycle 4	(490.0, 132.0 Da)	0.000
M_3	(500.0, 130.0 Da)	Active Symbiosis	0	Cycle 0	(500.0, 130.0 Da)	0.000
M_4	(250.0, 65.0 Da)	Accumulation / Resonance	$\lceil (450 - 250)/70 \rceil = 3$	Cycle 3	(460.0, 80.0 Da)	0.000
M_5	(900.0, 190.0 Da)	Thermal Dissipation	$\lceil (900 - 550)/90 \rceil = 4$	Cycle 4	(540.0, 142.0 Da)	0.000
M_6	(480.0, 115.0 Da)	Active Symbiosis	0	Cycle 0	(480.0, 115.0 Da)	0.000
M_7	(550.0, 140.0 Da)	Active Symbiosis	0	Cycle 0	(550.0, 140.0 Da)	0.000

where the intrinsic self-regulation operator Ψ is defined by the following 4×1 block vector:

$$\Psi(\mathbf{Z}_i) = \begin{pmatrix} u(E_i) \\ v(E_i) \\ -\mathbf{\Gamma}_i \mathbf{I}_i^{-1} \mathbf{J}_i \Delta t + \boldsymbol{\tau}_{\text{corr}}(E_i) \\ \mathbf{v}_i \Delta t \end{pmatrix} \quad (28)$$

Here $\mathbf{\Gamma}_i$ is held fixed during this intrinsic update, while $\boldsymbol{\tau}_{\text{corr}}(E_i)$ is an internal restoring torque:

$$\boldsymbol{\tau}_{\text{corr}}(E_i) = -\kappa_{\text{rot}} \text{sgn}(E_i - E_{\text{opt}}) \frac{\mathbf{J}_i}{\|\mathbf{J}_i\| + \varepsilon_0}. \quad (29)$$

The mutual coupling tensor $\boldsymbol{\Omega}_{ij}$ accounts for inter-subunit hydrodynamic and electrostatic interactions:

$$\boldsymbol{\Omega}_{ij} = \begin{pmatrix} -\nabla_{\mathbf{q}_i} V_{\text{pot}}(\|\mathbf{q}_i - \mathbf{q}_j\|) \cdot \mathbf{v}_i \Delta t \\ 0 \\ (\mathbf{q}_i - \mathbf{q}_j) \times \mathbf{F}_{ij}^{\text{hydro}} \Delta t \\ \mathbf{O}_{3 \times 3} \\ \mu_{ij}^{\text{Oseen}} \mathbf{F}_j^{\text{ext}} \Delta t \end{pmatrix}, \quad (30)$$

where $\mu_{ij}^{\text{Oseen}} = \frac{1}{8\pi\eta r_{ij}} (\mathbf{I} + \hat{\mathbf{r}}_{ij} \hat{\mathbf{r}}_{ij}^T)$ is the hydrodynamic Oseen tensor.

5 Computational Complexity Scaling

Traditional molecular modeling methodologies require extensive numerical integration:

- **Classical Molecular Dynamics (MD):** Requires integrating Newton’s equations via Verlet-type algorithms with time steps $\Delta t \sim 10^{-15}$ s. For an assembly requiring relaxation over t_{sim} , the step count is $S_{\text{MD}} = t_{\text{sim}}/\Delta t \sim 10^6 - 10^9$. The pairwise non-bonded force evaluation scales as $O(N^2)$ (or $O(N \log N)$ with Particle Mesh Ewald).
- **Markov Chain Monte Carlo (MCMC):** Requires $S_{\text{MC}} \sim 10^7$ stochastic trial configurations with acceptance ratio evaluations $P = \min(1, e^{-\beta \Delta E})$, yielding complexity $O(S_{\text{MC}} \cdot N^2)$.

Theorem 3 (Algorithmic Complexity of Symbiosis Engine). *For an uncoupled ensemble of N elements, the determination of all relaxation times K_i and asymptotic states $\mathbf{x}_i^{(\infty)}$ has temporal complexity:*

$$\mathcal{C}_{\text{uncoupled}} = O(N), \quad (31)$$

with spatial memory complexity $O(N)$. For an explicitly coupled network evaluated across iterative cycles, the complexity is:

$$\mathcal{C}_{\text{coupled}} = O(K_{\text{total}} \cdot N^2). \quad (32)$$

Proof. Evaluating (12) requires exactly one division, one ceiling operation, and one conditional branch per subunit, executing in $O(1)$ arithmetic operations. For N subunits, total time is $\sum_{i=1}^N O(1) = O(N)$. If a particular benchmark has a measured bound $K_{\text{total}} \ll S_{\text{MD}}$, the corresponding operation-count ratio is:

$$\rho = \frac{\mathcal{C}_{\text{MD}}}{\mathcal{C}_{\text{symb}}} \sim \frac{S_{\text{MD}} N^2}{K_{\text{total}} N^2} = \frac{S_{\text{MD}}}{K_{\text{total}}} \sim 10^6 - 10^7, \quad (33)$$

This expresses an operation-count comparison under the stated benchmark assumptions; it does not by itself establish a wall-clock speedup for a particular implementation. $\square$

6 Conditional Lyapunov Analysis of Coupled Consensus Dynamics

The coupled model requires a distinction between the finite-time absorption property of the uncoupled dead-band map and the consensus dynamics induced by the graph Laplacian. In particular, the Laplacian has a zero eigenvalue associated with the consensus direction. Therefore the coupling term alone contracts disagreement modes but does not, in general, force the consensus value to E_{opt} . The following result states the corresponding Lyapunov property without imposing an unsupported global convergence claim.

Definition 2 (Coupled Interaction Model). *Let the energy state vector be $\mathbf{E} = (E_1, E_2, \dots, E_N)^T \in \mathbb{R}^N$. The discrete update equation is*

$$\mathbf{E}^{(k+1)} = \mathbf{E}^{(k)} + \mathbf{U}(\mathbf{E}^{(k)}) - \gamma \mathbf{L} \mathbf{E}^{(k)}, \quad (34)$$

where $\mathbf{U}(\mathbf{E}) = (u(E_1), \dots, u(E_N))^T$, $\gamma > 0$ is the coupling gain, and $\mathbf{L} = \mathbf{D}_{\text{deg}} - \mathbf{W}$ is the Laplacian of a connected undirected graph, so that $\mathbf{L} = \mathbf{L}^T \succeq 0$ and $\lambda_1(\mathbf{L}) = 0$.

Proposition 1 (Consensus-Mode Contraction). *Consider the coupling-only dynamics*

$$\mathbf{E}^{(k+1)} = (\mathbf{I} - \gamma \mathbf{L}) \mathbf{E}^{(k)} \quad (35)$$

with a connected undirected graph. If

$$0 < \gamma < \frac{2}{\lambda_{\max}(\mathbf{L})}, \quad (36)$$

then every non-consensus Laplacian mode is contractive. More precisely, with

$$\mu_i = 1 - \gamma \lambda_i(\mathbf{L}), \quad (37)$$

we have $|\mu_i| < 1$ for every $i \geq 2$, whereas $\mu_1 = 1$. Hence the average energy is preserved by the coupling step and the disagreement component converges to zero.

Proof. Because $\mathbf{L}$ is symmetric, it admits the orthogonal spectral decomposition $\mathbf{L} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$, with $0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_N$. The eigenvalues of $\mathbf{I} - \gamma\mathbf{L}$ are $\mu_i = 1 - \gamma\lambda_i$. Condition (36) gives $-1 < \mu_i < 1$ for every $i \geq 2$. The consensus eigenvector is $\mathbf{1}$, for which $\mu_1 = 1$. Therefore the component orthogonal to $\mathbf{1}$ decays geometrically, while the consensus component is unchanged. Equivalently, $\mathbf{E}^{(k)}$ converges to $\bar{E} \mathbf{1}$, where $\bar{E} = N^{-1} \mathbf{1}^T \mathbf{E}^{(0)}$. $\square$

Proposition 2 (Invariance of the Symbiosis Box under a Sufficient Coupling Bound). *Let*

$$\mathcal{B}_{\text{symb}} = \{\mathbf{E} \in \mathbb{R}^N : |E_i - E_{\text{opt}}| \leq \epsilon, i = 1, \dots, N\}. \quad (38)$$

If the graph has maximum degree $d_{\max}$ and

$$0 < \gamma \leq \frac{1}{d_{\max}}, \quad (39)$$

then the coupling matrix $\mathbf{P} = \mathbf{I} - \gamma\mathbf{L}$ is nonnegative and row-stochastic. Consequently, $\mathcal{B}_{\text{symb}}$ is invariant under the coupling-only step. If the dead-band controller is zero throughout the box, the full update coincides with this coupling step while the trajectory remains in $\mathcal{B}_{\text{symb}}$.

Proof. For an undirected graph, $P_{ii} = 1 - \gamma d_i \geq 0$ under (39), while $P_{ij} = \gamma w_{ij} \geq 0$ for $i \neq j$. Each row sums to one because $\mathbf{L}\mathbf{1} = 0$. Thus each updated component is a convex combination of the previous components. A convex combination of values in $[E_{\text{opt}} - \epsilon, E_{\text{opt}} + \epsilon]$ remains in the same interval, proving invariance of $\mathcal{B}_{\text{symb}}$. $\square$

Remark 1. The two propositions separate two properties that were previously combined. The dead-band map provides finite-time absorption for the uncoupled dynamics. The Laplacian coupling provides asymptotic contraction of disagreement modes under the spectral condition (36). To conclude finite-time entry into $\mathcal{B}_{\text{symb}}$ for the fully coupled system, additional assumptions on the interaction term and initial conditions are required. Likewise, convergence to the specific value E_{opt} requires control of the consensus component; coupling alone preserves the mean and therefore does not provide such convergence in general.

7 Application to Biomolecular Distance Geometry and Folding

7.1 Euclidean Distance Matrix (EDM) Formulation

In structural bioinformatics, the complete tertiary conformation of a polypeptide or DNA macromolecule with n atoms/residues is completely specified by its Euclidean Distance Matrix $\mathbf{D} \in \mathbb{R}^{n \times n}$, where:

$$D_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|_2^2, \quad \forall i, j \in \{1, \dots, n\}. \quad (40)$$

A matrix $\mathbf{D}$ is an admissible EDM if and only if:

1. $D_{ii} = 0$ and $D_{ij} = D_{ji} \geq 0$;
2. The geometric centering matrix $\mathbf{G} = -\frac{1}{2}\mathbf{J}_n\mathbf{D}\mathbf{J}_n$ (where $\mathbf{J}_n = \mathbf{I}_n - \frac{1}{n}\mathbf{1}\mathbf{1}^T$) is positive semidefinite ($\mathbf{G} \succeq 0$) with $\text{rank}(\mathbf{G}) \leq 3$ [5].

7.2 Deterministic Symbiosis Contact Relaxation

Instead of relying on deep neural network probabilistic attention maps (e.g., Evoformer blocks in AlphaFold [1]), the Symbiosis Engine relaxes an initial trial distance matrix $\mathbf{D}^{(0)}$ directly toward physical van der Waals and covalent contact bands:

$$\mathcal{I}_{ij}^{\text{bond}} = [(d_{ij}^{\text{target}} - \epsilon_{ij})^2, (d_{ij}^{\text{target}} + \epsilon_{ij})^2], \quad (41)$$

The distance evolution equation follows:

$$\mathbf{D}^{(k+1)} = \Pi_{\mathbb{E}^3} \left(\mathbf{D}^{(k)} + \mathcal{T}_{\text{dist}} \left(\mathbf{D}^{(k)} \right) \right), \quad (42)$$

where $\Pi_{\mathbb{E}^3}$ denotes a nearest-point projection onto the set of admissible 3D Euclidean distance matrices. Because the rank-3 constraint is nonconvex, the nearest point need not be unique; a deterministic tie-breaking rule is therefore part of the numerical specification:

$$\Pi_{\mathbb{E}^3}(\mathbf{D}) \in \arg \min_{\hat{\mathbf{D}} \in \text{EDM}_3} \|\mathbf{D} - \hat{\mathbf{D}}\|_F^2. \quad (43)$$

The 3D Cartesian coordinates $\mathbf{R} = [\mathbf{r}_1, \dots, \mathbf{r}_n]^T \in \mathbb{R}^{n \times 3}$ are extracted via Classical Multidimensional Scaling (MDS) from the spectral decomposition of $\mathbf{G}$, after retaining the positive eigenvalues associated with the three-dimensional embedding and applying a deterministic eigenvector sign convention:

$$\mathbf{G} = \mathbf{V}_3 \mathbf{\Lambda}_3 \mathbf{V}_3^T \implies \mathbf{R} = \mathbf{V}_3 \mathbf{\Lambda}_3^{1/2}. \quad (44)$$

This defines a deterministic projection-contraction procedure. A claim of convergence within a fixed number of global matrix sweeps, or a claim of reduced wall-clock cost relative to another method, requires a separate numerical benchmark and is therefore not asserted here as a general theorem.

8 Conclusion

This study formulated and verified the *Deterministic Symbiosis and Molecular Self-Regulation Engine*. The mathematical framework delivers:

1. A fully deterministic, zero-deviation ($\Delta_{\text{dev}} = 0$) state operator $\mathcal{T}$ that strictly avoids limit cycles when $2\epsilon \geq \max(\Delta E_{\text{inc}}, \Delta E_{\text{dec}})$.
2. An analytical closed-form formula for the relaxation cycle count K_i , validated across a 7-element benchmark with a maximum individual convergence horizon of $K_{\text{total}} = 4$, with dynamic perturbation recovery in $K_{\text{pert}} = 2$.
3. A tensorial generalization incorporating angular momentum vectors $\mathbf{J}$ and hydrodynamic damping $\mathbf{\Gamma}$.
4. An $O(N)$ closed-form evaluation for uncoupled relaxation indices, together with a conditional Lyapunov analysis of the coupled consensus dynamics.
5. A deterministic EDM projection formulation whose convergence and structural accuracy can be assessed by separate numerical experiments.

The proposed engine provides a deterministic, mathematically transparent framework whose analytical properties and computational performance can be tested independently of probabilistic or heuristic methods. The present manuscript distinguishes finite-time absorption of the uncoupled dead-band map, asymptotic contraction of disagreement modes under Laplacian coupling, and numerical EDM reconstruction as separate claims with separate evidentiary status.

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