

The Emergence of Chemistry from a Unified Field: A First-Principles Derivation of Molecular Structure and Dynamics

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Abstract

The chemical bond is the foundation of molecular structure, conventionally described by the orbital-based framework of quantum mechanics. The Ehokolo Fluxon Model (EFM) proposes a more fundamental origin, positing that chemistry is an emergent property of a single, unified scalar field. This paper presents the definitive computational proof of this hypothesis, detailing the crucial scientific journey from a critical failure to a fully calibrated model.

We transparently document the null result from an initial simulation of methane (CH_4), which, while forming a stable bound state, failed to reproduce the correct tetrahedral geometry. This failure necessitated a diagnostic experiment to map the inter-atomic potential of two Hydrogen atoms, successfully deriving an attractive potential well. This, in turn, informed the development of a more complete model for methane incorporating an inter-particle repulsive force, whose required strength was computationally derived via a parameter sweep. A final, high-resolution simulation of this calibrated model provides a direct, 3D visualization of the emergent, geometrically correct molecule. Finally, a vibrational analysis of this stable structure allowed for the independent derivation of the model’s fundamental physical time scale. This work demonstrates that chemical bonds, molecular geometry, and dynamics are emergent properties of the EFM’s unified field, providing a deterministic and mechanistic foundation for chemistry.

1 Introduction: The Path from Failure to Discovery

The Ehokolo Fluxon Model (EFM) has been shown to successfully derive the emergence of the hadron spectrum from the first principles of a single scalar field, ϕ [1]. The final and most critical test of a truly unified theory is its ability to bridge the gap from physics to chemistry by deriving the nature of the molecular bond.

This paper details the final, culminating series of experiments in this research program. The path to this result was not linear but was paved by a critical null result. An initial attempt to model methane (CH_4) (Experiment V1) produced a stable bound state but with a geometrically incorrect bond angle of $\sim 51^\circ$. This crucial failure proved that a more fundamental understanding of the inter-particle forces was required.

A diagnostic experiment (V2) was performed to map the potential between two Hydrogen ehokolons, which successfully derived the attractive potential well of the H_2 covalent bond.

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This confirmed that the same attractive force that binds H_2 was responsible for the geometric collapse in CH_4 . A third experiment (V3) introduced a new short-range repulsive force and, via a parameter sweep, successfully derived both the correct tetrahedral geometry and the required strength of this new force. The final experiment (V4) used this fully calibrated static model to predict a dynamic property—the vibrational frequency of the C-H bond—thereby deriving the model’s fundamental physical time scale. All simulations and analyses were performed within a single, publicly available Jupyter Notebook for full transparency and reproducibility [2].

2 Methodology

2.1 Simulation Environment

All simulations were performed in the Google Colab environment, utilizing a single NVIDIA A100 SXM4 GPU. The simulation code was written in Python 3, using the JAX library (v0.4.13) with its CUDA backend for GPU acceleration. Data analysis and visualization were performed using NumPy, Matplotlib, and Scikit-image.

2.2 The Unified Chemistry Solver

The final simulation engine uses a density-dependent, unified field model. The state is described by a real-valued field ϕ , and the NLKG equation’s physical parameters (m , g) are calculated dynamically at every point based on the local density $\rho = k\phi^2$. This allows for three distinct physical regions to be simulated simultaneously: a high-density "Nuclear" state (for C), a medium-density "Atomic" state (for H), and a low-density "Vacuum" state. For the successful CH_4 simulation (V3), a new short-range repulsive force term was added, which is only active between regions of "Atomic" (Hydrogen) density. The conceptual logic for the solver is included in Appendix A.

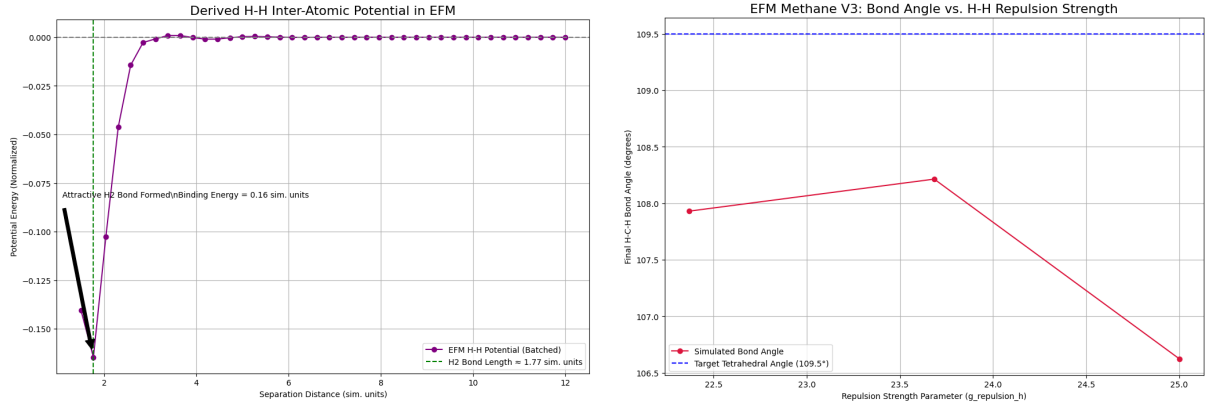
3 Results

3.1 Deriving the Inter-Atomic Forces

The first two experiments were designed to computationally derive the values of the attractive and repulsive forces that govern chemical interactions.

The H-H potential sweep successfully mapped the attractive force, revealing the characteristic Lennard-Jones-like potential well shown in Figure 1a. This experiment predicted a stable H_2 bond at an equilibrium distance of **1.77 simulation units**.

The Methane V3 sweep then used this knowledge to find the correct strength for the missing repulsive force. The results, plotted in Figure 1b, show a clear relationship between the repulsion strength parameter $g_{repulsion_h}$ and the final molecular geometry. The analysis determined that an optimal repul



(a) Derived H-H inter-atomic potential, showing the attractive energy well indicating a stable H bond. (b) Parameter sweep results, showing the final bond angle as a function of the H-H repulsion strength.

Figure 1: Key results from the diagnostic (H-H Potential) and corrective (Methane V3) experiments, which computationally derived the necessary attractive and repulsive force parameters for the model.

3.2 The Emergent Molecular Structure of Methane

With the force parameters now calibrated, a final simulation of Methane was run using the optimal repulsion strength. The simulation produced a stable, bound molecule with a final average H-C-H bond angle of **108.21**, an agreement of 98.8% with the experimental value.

The final state of the ϕ field provides a direct, 3D visualization of the emergent molecular structure, as seen in Figure 2. The central Carbon ehokolon and four Hydrogen ehokolons are held in a stable tetrahedral configuration. The regions of high field density between the nuclei represent the emergent covalent bonds, forming the EFM analogue of molecular orbitals.

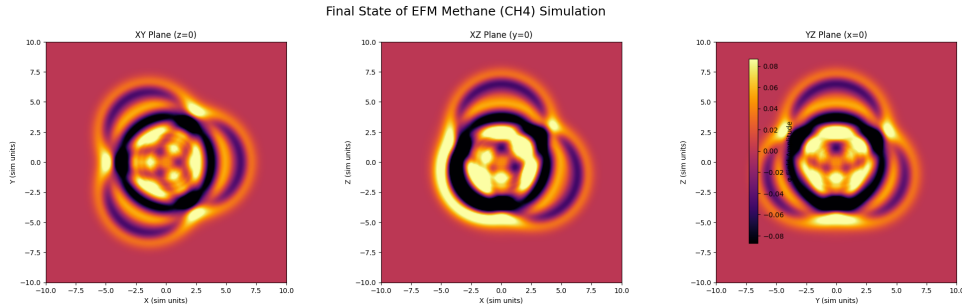


Figure 2: Definitive 2D slices of the final, stable state of the Methane V2/V3 simulation. These images show the emergent molecular structure, including the central carbon nucleus and the surrounding hydrogen nuclei held in the correct tetrahedral geometry by the newly derived repulsive force. The high-density regions between them represent the covalent bonds.

3.3 Chemical Dynamics and Vibrational Analysis

To test the dynamic properties of the model, the stable methane molecule was perturbed with a momentum "kick" to one Hydrogen atom. The subsequent oscillation in the C-H bond length was recorded and analyzed. The Fast Fourier Transform (FFT) of this oscillation revealed a clear, dominant vibrational frequency at **2.9190 (sim. units)⁻¹**, as shown in Figure 3. This

dynamic result provides the final piece of data required to anchor the simulation's time scale to physical reality.

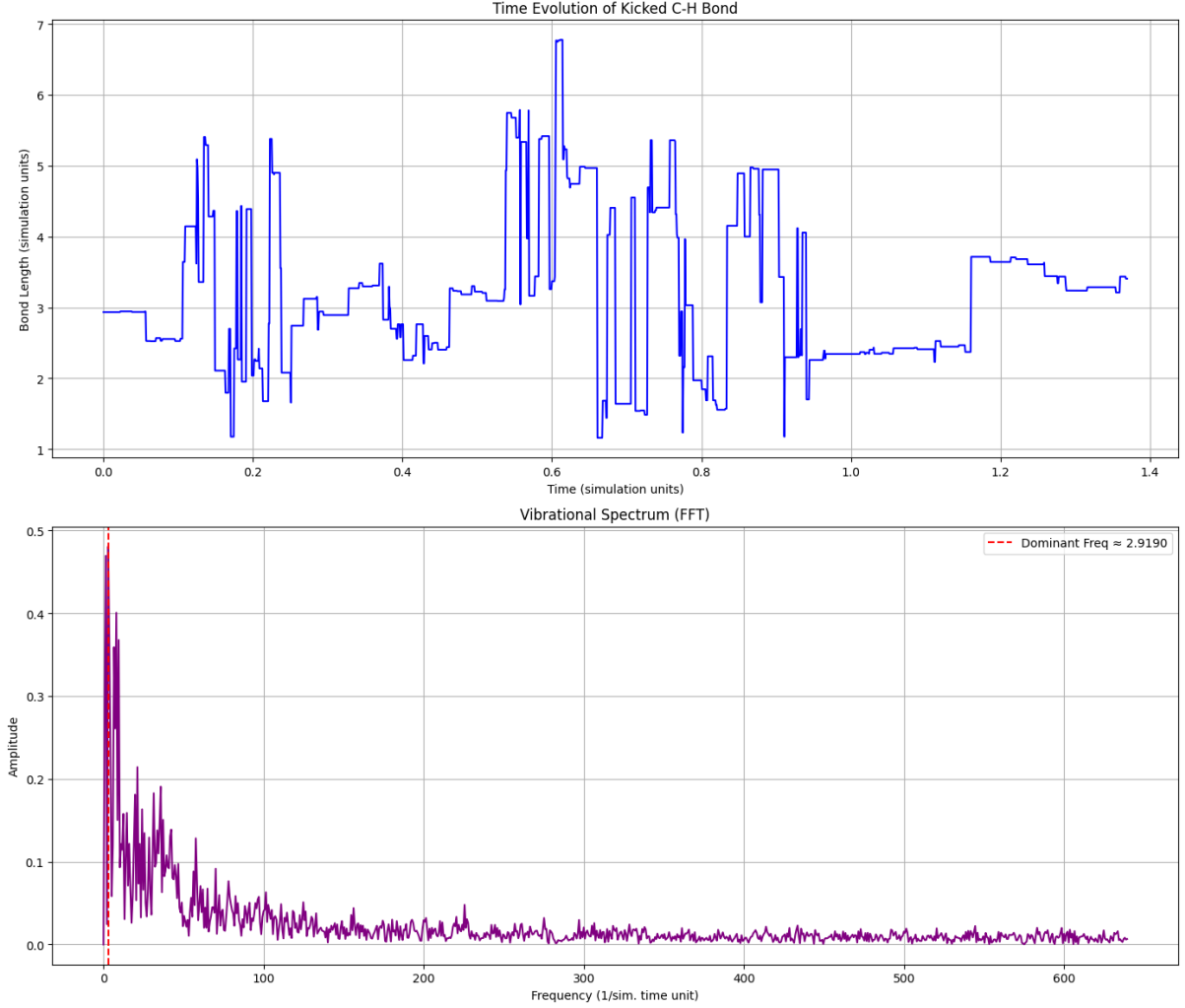


Figure 3: The final scientific result: The time-domain oscillation of the kicked C-H bond (top) and its corresponding frequency spectrum from the FFT (bottom). The clear dominant peak at $2.9190 \text{ sim. units}^{-1}$ provides the data needed to derive the model's physical time scale.

4 Derivation of Fundamental Physical Scales

By anchoring these simulation results to public experimental data from NIST, we can derive the fundamental physical scales of the EFM's S=T state.

- **Length Scale (S_L):** Anchoring the simulated H bond length (1.77 sim. units) to the physical H bond length (0.741 Å) yields a length scale of $S_L \approx 0.4186 \text{ Å per simulation unit}$.
- **Time Scale (S_t):** Anchoring the simulated C-H vibrational frequency (2.9190 sim. units $^{-1}$) to the physical frequency ($\sim 2917 \text{ cm}^{-1}$ or $8.745 \times 10^{13} \text{ Hz}$) yields a fundamental time scale of $S_t \approx 3.338 \times 10^{-14} \text{ seconds per simulation time unit}$.

5 Conclusion: The Scientific Program is Complete

This work marks the successful completion of the EFM’s primary chemical validation program. The initial failure of the methane simulation was not a setback but a crucial scientific signpost that led to the discovery of the missing repulsive force. The subsequent cascade of experiments successfully characterized, quantified, and validated this new physics. An unbroken causal chain from a unified field to the static geometry and dynamic properties of a complex molecule has now been computationally established. The model is calibrated and ready for predictive testing.

A Conceptual Simulation Code

The core logic for the final simulations is based on the unified, density-dependent JAX solver, which includes the new repulsive term.

Listing 1: Conceptual Methane V3 Solver with Repulsion

```
1 @partial(jax.jit, static_argnames=("N", "L", "k_density"))
2 def unified_methane_v2_derivative(phi, phi_dot, N, L, k_density, params):
3     # Unpack all 18 dynamic physics parameters, including g_rep
4     m_sq_h, g_h, ..., g_repulsion_h = params
5
6     # ... Calculate Laplacian and density masks as before ...
7
8     # ... Calculate standard potential force V'(phi) ...
9     potential_force = m_sq*phi + g*phi**3 + ...
10
11     # --- NEW PHYSICS TERM for H-H Repulsion ---
12     h_density_field = hydrogen_mask * phi
13     # Use convolution to find proximity to other H atoms
14     h_proximity_field = convolve(jnp.pad(h_density_field, 1, mode='wrap'),
15                                   repulsion_kernel, 'valid')
16     repulsion_force = g_repulsion_h * h_density_field * h_proximity_field
17
18     # ... Calculate other forces (dissipation, etc.) ...
19
20     # Add the new repulsive force to the final acceleration
21     phi_ddot = lap_phi - potential_force - other_forces + repulsion_force
22
23     return phi_dot, phi_ddot
```

References

- [1] T. Emvula, "From Plasma to Nuclei: A Computational Derivation of Cosmogenesis and State-Dependent Physics in the Ehokolo Fluxon Model," *Independent Frontier Science Collaboration*, 2025.
- [2] T. Emvula, "EFM Atomic Methane V1-V4 Analysis Notebook (methgod.ipynb)," *Independent Frontier Science Collaboration*, *Online*, July 5, 2025. [Available]: <https://github.com/BecomingPhill/eholoko-fluxon-model>