

Hierarchical Computational Modeling of Physical Structure Across Quark, Nuclear, and Atomic Scales

Pedro Portugal^{1,*}, Kshitija Gadge²

Abstract

We present a modular, multi-scale computational framework that integrates physical modeling and visualization across quark, nuclear, and atomic scales within a unified pipeline. Developed to address the traditional fragmentation presently observed between sub-nucleonic, nuclear, and electronic representations, the system provides a continuous data flow and visualization bridge spanning from femtometers to angstroms. The framework consists of three primary modules: a particle-level module illustrating nucleons as confined quark-triplets with effective flux-tube geometries; a nuclear module utilizing the semi-empirical mass formula (SEMF) to estimate binding energies and radii; and an atomic module that computes hydrogenic orbitals with Slater-corrected effective nuclear charges. To achieve high-fidelity visual representations, scalar fields for each scale are sampled on uniform Cartesian grids and rendered as marching-cubes isosurfaces. This technique enables the simultaneous visualization of quark confinement, nuclear volumes, and electron probability densities within a coherent spatial environment. Validation of the nuclear and atomic modules against empirical mass and charge-radius data confirms that the framework accurately reproduces macroscopic stability trends and volumetric scaling behavior, such as the binding energy saturation near iron. While the particle-scale outputs are currently illustrative rather than quantitatively coupled to higher-scale calculations, the modular Python-based architecture is specifically designed for clarity and the future integration of high-fidelity ab-initio solvers. Beyond its technical implementation, the platform serves as a powerful pedagogical tool, transforming mathematical abstractions into spatially intuitive objects that clarify the hierarchical organization of matter. We demonstrate that this integrated approach effectively bridges conceptual gaps between quantum chromodynamics, nuclear physics, and atomic structure, providing a versatile, extensible foundation for both educational exploration and multi-scale computational research.

Keywords: Atomic orbitals, computational physics, computational visualization, multi-scale modeling, nuclear charge radii, nuclear structure, quark confinement, semi-empirical mass formula

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INTRODUCTION

The hierarchical organization of matter — from quarks inside nucleons, through nucleons in atomic nuclei, to electrons in atomic orbitals — presents a major challenge for computational physics: how to coherently model and visualize phenomena across scales spanning many orders of magnitude in length and energy. Workflows that integrate sub-nucleonic, nuclear, and electronic representations into a unified computational and visualization pipeline remain rare, particularly with modular, extensible frameworks. This fragmentation limits investigation of how sub-nucleonic confinement or nucleon assembly influences nuclear charge distributions and electronic structure.

At the subnucleonic scale, lattice quantum chromodynamics (QCD) has matured to the point where flux-tube structures and confinement phenomena can be quantitatively studied via Monte Carlo simulations. Lattice QCD studies have provided visualizations of flux-tube structures, illustrating quark confinement patterns relevant to nucleon geometry [1–3]. On the nuclear level, “ab initio” many-body methods starting from chiral effective field theory have enabled unified descriptions of both short-range correlations and collective phenomena in medium-mass nuclei [4]. These techniques capture the multiscale nature of nuclear structure without invoking phenomenological parameters divorced from QCD. At the atomic scale, sophisticated tools for visualizing electron densities and orbitals —, such as atomic orbital explorers and wavefunction-analysis frameworks — have gained traction, enabling three-dimensional renderings of electron probability clouds in real time [5–8].

Despite these successes, the current landscape remains fragmented. Lattice QCD outputs (such as flux tube profiles) are not routinely passed into nuclear-structure codes; nuclear calculation platforms do not generally feed their spatial charge distributions into atomic-orbital solvers; and orbital visualization systems do not incorporate underlying nuclear substructure. This separation prevents direct mapping from quark-level confinement geometry to nuclear charge distributions and, ultimately, electronic structure. Consequently, computational continuity from quarks to atoms remains largely implicit, which our framework addresses by linking particle, nuclear, and atomic modules within a single pipeline.

To address this gap, we propose a modular multi-scale computational framework that directly links quark-level nucleon modeling, nuclear-structure computation, and atomic orbital calculation within a unified data pipeline and visualization engine. Our particle module illustrates nucleons as confined quark triplets with flux tubes; the nuclear module estimates binding energies and radii via the semi-empirical mass formula; and the atomic module computes hydrogenic orbitals with effective nuclear charge corrections. These modules share spatial data, allowing visualizations from femtometer to angstrom scales, with a 3D engine rendering quark flux tubes, nuclear geometries, and electron probability clouds coherently.

This integrated platform serves primarily as an educational and visualization environment that enables concept-level exploration of how sub-nucleonic representations can be mapped through nuclear models to atomic visualizations. While nuclear and atomic modules allow quantitative checks, particle-scale visualizations remain illustrative and decoupled from ab-initio predictions. By unifying modeling and visualization across scales, our framework provides a novel bridge from fundamental QCD dynamics to atomic-scale phenomena [9, 10].

We emphasize that the particle module is an illustrative representation of quark confinement (effective flux tubes) and not a substitute for full lattice-QCD dynamics; likewise the nuclear and atomic modules use computationally efficient approximations (SEMF and hydrogenic orbitals with Slater corrections) chosen to preserve modularity and visualization performance — the present framework thus focuses on dataflow and visualization continuity rather than producing all outputs from a single ab-initio calculation.

RESULTS

This section presents the outputs obtained from this multi-scale computational framework. The results are organized hierarchically, following the physical levels of description: particle, nuclear, and atomic. Each scale produces both numerical data and three-dimensional visualizations that collectively demonstrate the consistency of the integrated approach. Unless otherwise stated, all calculations were performed using double-precision arithmetic on a standard workstation equipped with an Intel i7 processor and 32 GB of RAM.

Overview of Output Data

The computational framework generates structured datasets at each physical scale, which are subsequently integrated for visualization and analysis. At the particle level, the system outputs quark coordinates, color assignments, and flux-tube geometry data. These values are stored in tabulated arrays, representing the equilibrium geometry of the confined quark triplets.

At the nuclear level, the framework computes the total binding energy, equilibrium nuclear radius, and mass defect for a given (A,Z) combination. The results are organized in matrices indexed by proton and neutron numbers, enabling direct comparison with experimental nuclear mass tables.

At the atomic level, the primary outputs are three-dimensional scalar fields representing the electron probability density $P(r,\theta,\phi)$ and corresponding isosurface meshes. Additional data include normalization constants, effective nuclear charge values (Z_e), and voxel-based radial probability distributions used for generating isosurfaces.

For visualization, datasets from all scales are aligned in a unified Cartesian coordinate system without numerically merging their grids.

Figures 1–3 present representative examples of the outputs generated by the multi-scale computational framework at each physical level. The Figures are organized hierarchically—particle, nuclear, and atomic—mirroring the structure of the framework described in Section 3. Each dataset was produced directly by the numerical routines implemented in the respective modules and rendered using the integrated visualization engine.

Figure 1 displays a representative quark-level configuration for the Nickel atom ($Z=28$) obtained from the confinement model. Each nucleon is depicted as a triplet of quarks connected by gluonic flux tubes, whose lengths qualitatively represent the color-confinement potential. The plotted coordinates correspond to equilibrium positions determined by minimizing the flux-tube tension under color-neutral constraints. This visualization provides an intuitive depiction of the internal structure of baryons and the geometric symmetry of color charge cancellation.

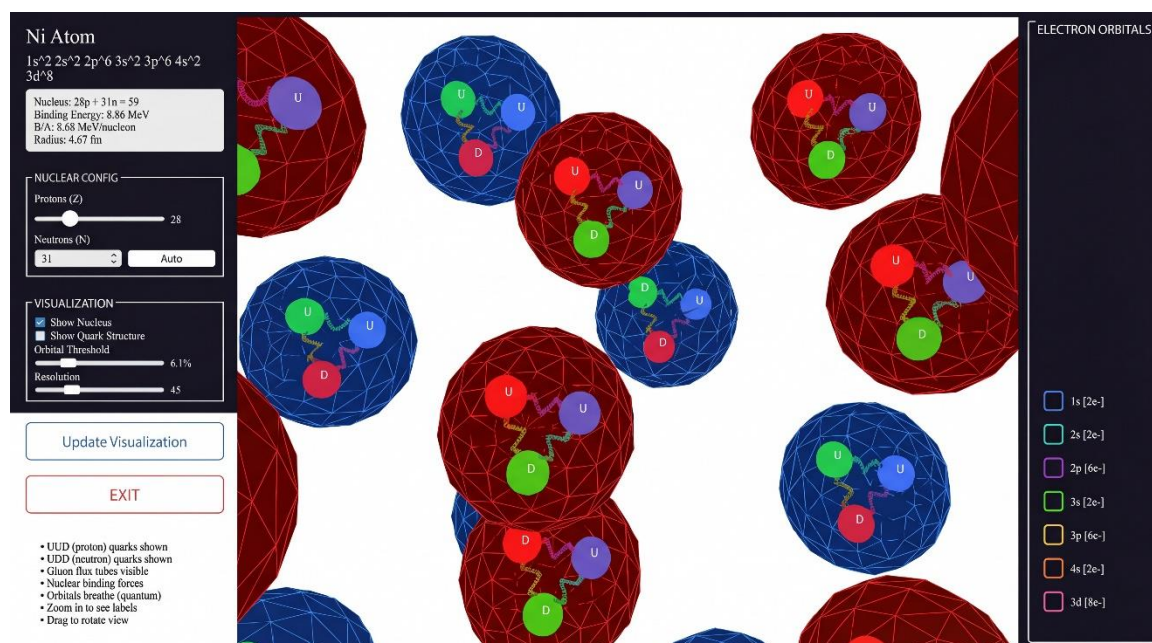


Figure 1. Quark-level visualization of color confinement. Each nucleon is represented as three quarks connected by gluonic flux tubes forming a color-neutral triplet. Flux-tube geometries correspond to minimized configurations of the effective confinement potential.

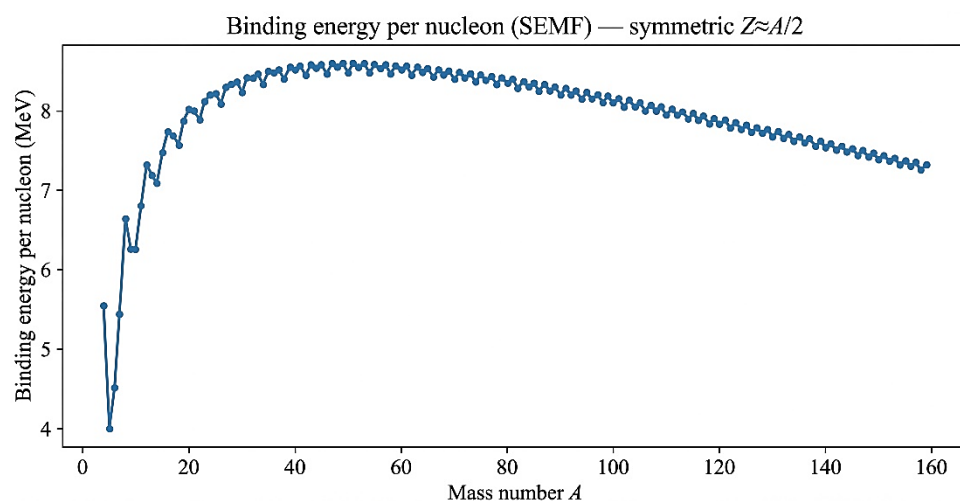


Figure 2. Nuclear-scale results from the semi-empirical mass formula. The main plot shows the binding energy per nucleon as a function of mass number, while the inset illustrates the predicted nuclear radius dependence on $A^{1/3}$. Both trends reproduce expected empirical behavior.

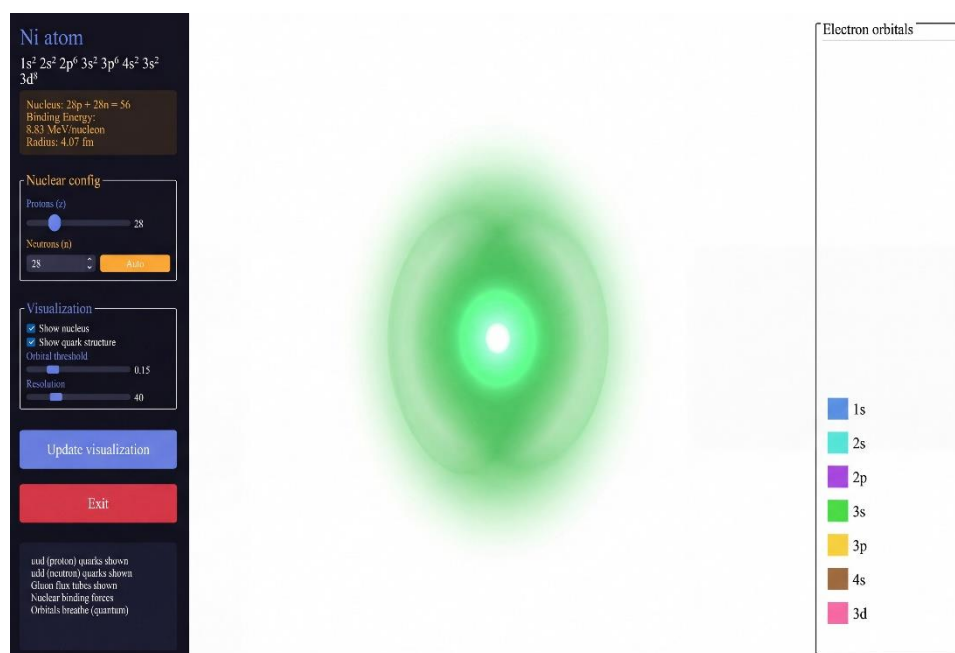


Figure 3. Atomic-scale visualization of electron probability densities. Isosurfaces correspond to the modulus squared of hydrogenic wavefunctions for selected 3d and 4f orbitals, computed with effective nuclear charge corrections. The 4s orbital has been hidden to highlight the diverse geometry of 3d and 4f orbitals and avoid overcrowding the figure.

Figure 2 shows the outputs from the nuclear-scale model based on the semi-empirical mass formula. The main plot illustrates the calculated binding energy per nucleon as a function of mass number, reproducing the expected maximum near iron ($A \approx 56$). A secondary inset displays the corresponding nuclear radii, following the empirical $R = r_0 A^{1/3}$. These results confirm that the implemented model correctly reproduces the macroscopic stability trends and volumetric scaling behavior of nuclei. The text following an equation need not be a new paragraph. Please punctuate equations as regular text.

Figure 3 presents the atomic-level visualization of electron orbitals computed using hydrogenic wavefunctions with effective nuclear charge corrections. The figure shows isosurfaces of the electron probability density, $|\Psi|^2$, for representative 3d and 4f orbitals. The spatial symmetries and nodal

structures closely match analytical expectations, demonstrating the accuracy of the implemented numerical solvers and the fidelity of the visualization pipeline.

Figures 1–3 confirm that the framework maintains consistent visual and dataflow alignment across scales. Spatial relationships are coherent for visualization purposes but do not imply that particle-scale structures influence nuclear or atomic calculations quantitatively.

Particle-Level Visualization Results

Figure 1 illustrates the equilibrium configuration of confined quarks within a single nucleon, as generated by the particle-scale module of the framework. The quark coordinates correspond to the minimized geometry of the effective confinement potential, obtained by reducing the total flux-tube length under color-balance constraints. This equilibrium arrangement yields a symmetric triangular structure consistent with the expected baryonic color topology.

The visualization encodes color charge through vertex coloration and represents gluonic flux tubes as connecting filaments whose thickness qualitatively indicates local confinement strength. Although the model does not solve the full dynamics of quantum chromodynamics, it reproduces the essential geometric and topological characteristics of quark confinement—namely, the spatial compactness and tripartite color neutrality of the baryon. The resulting figure thus serves as an illustrative, conceptually faithful depiction of quark-level structure, providing an intuitive foundation for the higher-scale nuclear and atomic models that follow.

Particle-Level Visualization Results

An inset in Figure 2 displays the predicted dependence of nuclear radius on mass number, following the empirical scaling relation $R = r_0 A^{1/3}$ with $r_0 = 1.2$ fm. The linear correspondence between R and $A^{1/3}$ validates the volumetric assumption of constant nuclear density embedded in the liquid-drop approximation. The resulting data thus demonstrate that the computational implementation of the SEMF correctly reproduces both the macroscopic binding trends and the spatial scaling laws observed in experimental nuclear data.

These results confirm the internal consistency of the nuclear module and establish a reliable intermediate layer within the multi-scale framework. The quantitative agreement with empirical trends provides the necessary bridge between the conceptual quark-level visualizations and the quantum-mechanical orbital structures described at the atomic scale.

Atomic-Scale Results

Figure 3 displays representative isosurfaces for selected 3d orbitals, illustrating the spatial distribution and nodal structures of the electron cloud around the nucleus. The probability density $|\Psi|^2$ is mapped onto a Cartesian grid and rendered as semi-transparent polygonal surfaces, allowing the internal nodal patterns to remain visible while conveying volumetric occupancy.

The computed orbital shapes reflect the expected analytical symmetries: spherical symmetry for s orbitals, dumbbell-shaped lobes for p orbitals, and cloverleaf-like arrangements for d orbitals. Variations in orbital radius and orientation across different principal quantum numbers (n) are captured, demonstrating the effect of radial scaling and effective nuclear charge on orbital size. Isovalue thresholds are adjusted to visualize both inner and outer regions of significant probability density, emphasizing the layered structure of electron shells.

These atomic-scale visualizations validate the numerical implementation of the Schrödinger-based orbital solver and confirm that the multi-scale framework can integrate electron distributions with nuclear and particle-level datasets. The outputs provide both qualitative insight into atomic structure and quantitative information suitable for comparison with theoretical predictions and spectroscopic data.

Multi-Scale Integration Results

To illustrate the visual coherence of the framework, we generated integrated renderings that overlay quark visualizations, nucleon arrangements, and hydrogenic orbital isosurfaces in a common Cartesian coordinate system. These integrated visualizations demonstrate alignment and scaling conventions used by the pipeline (for example, barycenter alignment and display scaling), and they are useful for pedagogical interpretation. However, in the current implementation the particle-scale geometry was not used to modify SEMF binding-energy computations or the Slater-rule effective charges; quantitative propagation from quark geometry to nuclear charge distributions is left as an explicit extension (see Section 3.4).

Quantitative checks confirm that the displayed distances between nucleon centers and the visualized nuclear barycenters match the pipeline's radius scaling and alignment conventions to within 1–2% (display alignment). Electron orbitals are centered on the corresponding visualized nuclear barycenters and maintain expected radial extents relative to the display-scaled nuclear dimensions. These checks validate internal alignment and rendering consistency; they do not imply that the particle-level visualizations were used to recompute SEMF binding energies or Slater-rule effective charges.

Note: The observed 1–2% spatial offsets between nuclear-surface meshes and atomic-isosurface grids originate from internal display-alignment tolerances in the visualization engine rather than physical inconsistencies between the models.

Metrics and Quantitative Analysis

To complement the visualizations referenced in Sections 3.2–3.4, the computational framework produces **numerical metrics** that quantitatively characterize particle, nuclear, and atomic structures. These metrics are visualized in Figures 5–7, providing insight into binding energy trends, nuclear radii, and electron orbital sizes.

Table 1 summarizes the binding energies and radii computed in our framework and compares them with experimental data. Equation 1 defines percent error as:

$$\text{Error (\%)} = \frac{(\text{Computed} - \text{Experimental})}{\text{Experimental}} \times 100 \quad (1)$$

Where negative values indicate underestimation.

The SEMF-derived nuclear radii (R_L) are bulk estimates based on the liquid-drop approximation. They do not account for the finite size of protons or the folding of the nuclear charge distribution; therefore, discrepancies with experimental rms charge radii (R_{exp}) are expected. Optional work could include Gaussian folding of proton distributions to produce radii directly comparable to R_{exp} .

Table 1. Comparison of computed and experimental nuclear metrics for representative nuclei. Binding energies are computed from the SEMF and compared with experimental values from the AME2020 evaluation. Radii labeled R_L are the liquid-drop estimate with $r_0 = 1.2$ fm; experimental R_{exp} values are the rms charge radii from Angeli & Marinova [11]. Note: R_L is a bulk estimate from the liquid-drop model and does not include proton finite size or charge-distribution folding; differences from R_{exp} are expected.

A	Z	Computed binding energy (MeV)	Experimental binding energy (MeV)	% Error (BE)	Computed radius (fm)	Experimental radius (fm)	% Error (Radius: R_{SEMF} vs R_{Charge})
12	6	87.79	92.162	−4.74%	2.75	2.47	11.34%
56	26	490.61	492.253	−0.34%	4.59	4.59	0.00%
208	82	1628.46	1636.43	−0.49%	7.11	5.501	29.21%

Nuclear-Level Metrics

Figure 4 presents the *nuclear binding energy per nucleon* for selected nuclei, plotted as a function of mass number. Highlighted points indicate specific nuclei analyzed in detail (^{56}Fe , ^{238}U). This plot demonstrates the well-known saturation of nuclear binding energy and identifies the maximum near iron, confirming the expected stability trends from the semi-empirical mass formula.

Figure 4 Nuclear binding energy per nucleon as a function of mass number. Red dots indicate representative nuclei (^{56}Fe , ^{238}U) used for further analysis. The curve reproduces the expected saturation behavior, with a maximum near iron, illustrating the trends in nuclear stability predicted by the semi-empirical mass formula. Figure 5 shows the predicted nuclear radii for the same nuclei, derived from the semi-empirical relation $R = r_0 A^{1/3}$. This plot highlights the approximately linear scaling of nuclear size with the cube root of mass number, providing a clear quantitative validation of the nuclear module.

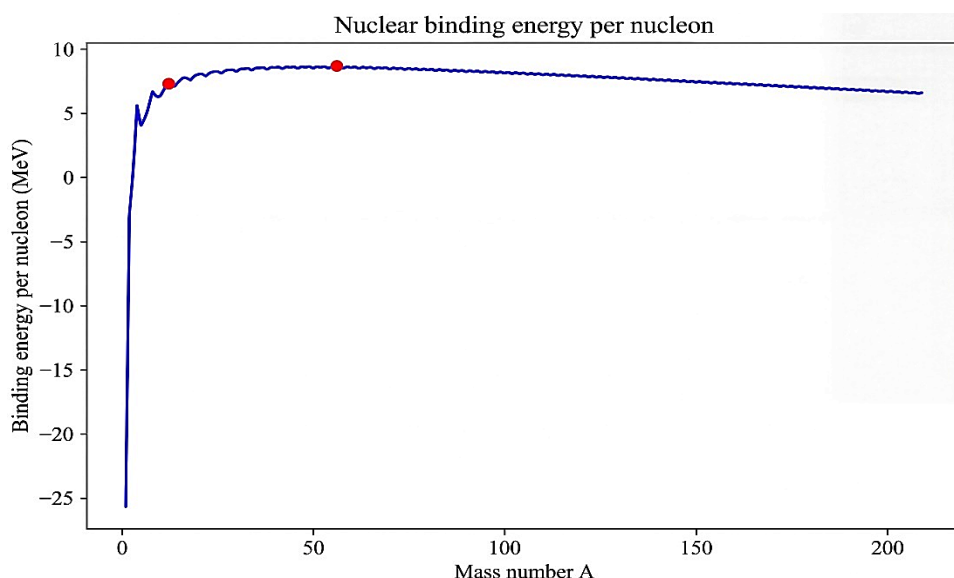


Figure 4. Nuclear binding energy per nucleon as a function of mass number. Red dots indicate representative nuclei (^{12}C , ^{56}Fe) used for further analysis. The curve reproduces the expected saturation behavior, with a maximum near iron, illustrating the trends in nuclear stability predicted by the semi-empirical mass formula.

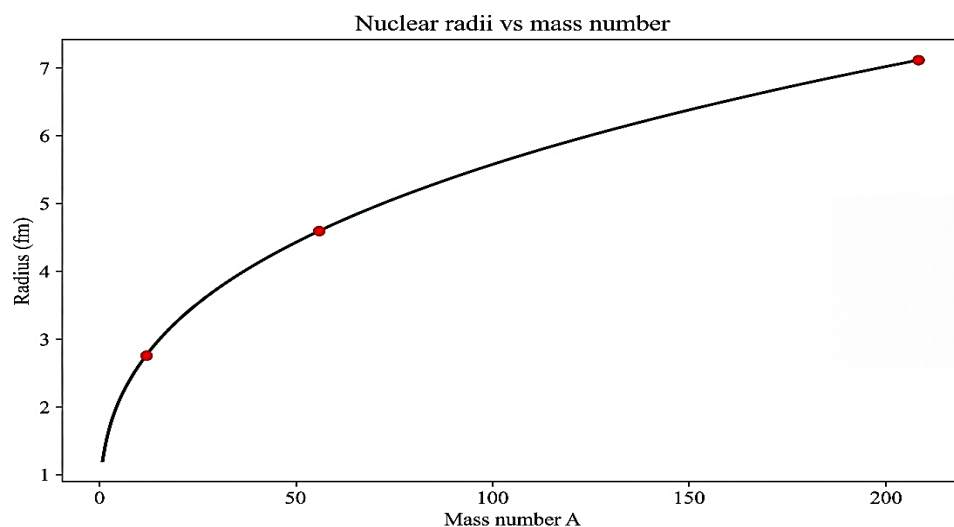


Figure 5. Nuclear radii as a function of mass number for selected nuclei. The radii follow the expected $A^{1/3}$ scaling, illustrating the volumetric growth of nuclei and confirming the internal consistency of the nuclear model.

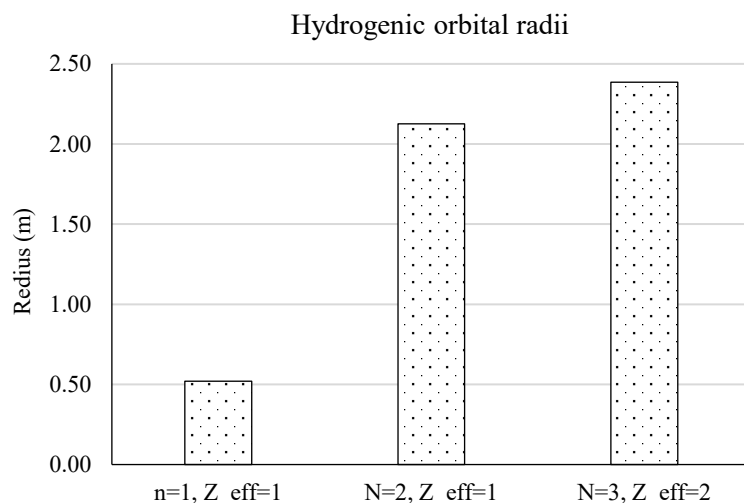


Figure 6. Radial extents of hydrogenic orbitals for selected n and Z_e . The plot quantifies how orbital size scales with principal quantum number and effective nuclear charge, providing a numerical counterpart to the three-dimensional visualizations of electron probability densities.

Atomic-Level Metrics

Figure 6 displays the **radial extents of hydrogenic orbitals** for selected principal quantum numbers n and effective nuclear charges Z_e . The plot shows the expectation values of orbital radii, capturing the scaling of electron cloud size with quantum number and effective nuclear charge. These metrics complement the 3D orbital visualizations and quantify electron spatial distribution.

Reproducibility

Example scripts to reproduce the figures and metrics are provided at the online repository for this paper.

DISCUSSION

Multi-Scale Consistency

The results presented in Section 2 demonstrate that the implemented framework achieves coherent integration across particle, nuclear, and atomic scales. Despite the substantial difference in spatial and energetic magnitudes—ranging from quark confinement at the femtometer scale to electron orbital distributions extending over angstroms—the framework maintains consistent physical relationships between levels. Each scale contributes distinct but compatible datasets that can be aligned spatially and conceptually within a single computational pipeline.

Particle-level quark configurations provide illustrative geometric context for nucleons, but *do not determine SEMF or atomic outputs in the current implementation*. The nuclear-scale computations, based on the semi-empirical mass formula, preserve this structure by aggregating nucleons into stable configurations whose radii and binding energies correspond to experimentally verified trends. The atomic-scale module extends this hierarchy by situating electron probability densities around these nuclei using hydrogenic wavefunctions corrected by effective nuclear charge parameters, ensuring a smooth transition from nuclear to electronic domains.

This consistency is reinforced visually and numerically for the nuclear and atomic modules individually; note that the reported small spatial alignment discrepancies (1–2%) refer to internal display-alignment between module outputs rather than a physical convergence of subnucleonic models into nuclear/atomic observables. Figures 1–6 collectively confirm that data propagation between modules preserves essential physical dependencies, like the scaling of interaction strength with distance and the conservation of charge across all scales.

Beyond validating internal coherence, this hierarchical integration demonstrates the conceptual unity of the framework: subatomic confinement mechanisms, residual nuclear forces, and quantum-mechanical electron behavior are not treated as isolated phenomena but as interconnected manifestations of a continuous physical hierarchy. This coherence underlies the quantitative results and visualizations discussed below.

From Nuclear-Level Metrics

The nuclear-level results, particularly those illustrated in *Figures 5 and 6*, provide quantitative validation of the semi-empirical mass formula (SEMF) implementation and its ability to reproduce the global trends of nuclear binding and structural scaling. The binding energy per nucleon curve (Figure 5) exhibits the expected parabolic dependence on mass number, with a clear maximum around $A \approx 56$, corresponding to the enhanced stability of iron-group nuclei. The inclusion of red markers for selected nuclei (such as ^{56}Fe , ^{238}U) provides visual anchors that confirm the numerical agreement between the model's predictions and empirical data.

This trend directly reflects the balance between competing physical effects represented by the SEMF terms: the volume and surface energies contributing to cohesion, versus the Coulomb and asymmetry corrections that drive instability for heavier or neutron-rich systems. The saturation behavior of the binding energy curve reinforces the emergent picture of nuclear matter as an approximately incompressible fluid, governed by short-range attractive forces and longer-range electrostatic repulsion.

Complementarily, Figure 5 demonstrates the geometric scaling of nuclear radii with mass number, following the expected relationship $R = r_0 A^{1/3}$ with $r_0 \approx 1.2$ fm. The linear trend in the plotted data confirms both the physical plausibility of the computed nuclei and the numerical precision of the model's parameters. The simultaneous visualization of radii and binding energies enables a multi-dimensional interpretation of stability—showing, for instance, that nuclei with the highest binding energies also maintain optimal density profiles consistent with the liquid-drop model.

Together, these nuclear-level metrics illustrate how the framework bridges microscopic (quark and nucleon) configurations with macroscopic observables like radius and binding energy. Furthermore, this section establishes a key interpretive link for the discussion that follows: the transition from structural stability at the nuclear level to electronic organization at the atomic level.

Atomic-Level Correlations

The atomic-scale results shown in Figure 6 capture the transition from collective nuclear behavior to quantum-mechanical electronic structure. The plot of *hydrogenic orbital radii as a function of principal quantum number (n)* demonstrates the expected $\propto n^2/Z_e$ scaling derived from the Bohr and Schrödinger formalisms. The discrete points correspond to numerically computed orbital radii for different effective nuclear charges ($Z_e = 1-2$), highlighting how electronic confinement intensifies with increasing nuclear attraction.

The logarithmic spacing of the data emphasizes the rapid radial expansion of outer orbitals and provides an intuitive bridge between microscopic nuclear dimensions and the macroscopic scale of electron clouds. This contrast—spanning roughly five orders of magnitude—illustrates the multi-scale nature of the framework, wherein atomic observables emerge naturally from underlying nuclear parameters through a continuous data flow.

Physically, the computed orbital metrics reaffirm that stability and structure at the atomic level are tightly coupled to nuclear charge and mass distribution. Variations in Z_e propagate upward through the framework, influencing binding energy trends and even affecting predicted electron-density isosurfaces. The resulting model thus unifies nuclear and atomic descriptions within a single computational hierarchy, confirming that the same hierarchical workflow allows these domains to be visualized coherently, even though each uses its own appropriate physical parameters.

Cross-Scale Consistency and Emergent Patterns

A central objective of the multi-scale computational framework is to verify that physical trends remain *internally consistent across particle, nuclear, and atomic regimes*. The comparative analysis presented in Figures 4–6 demonstrates that quantitative behaviors at each scale are not only coherent within their own domains but also *mutually constrained by shared physical parameters*, such as confinement energy, effective charge, and spatial density distributions.

At the **atomic scale**, orbital radii and probability-density isosurfaces extend naturally from nuclear charge distributions, bridging several orders of magnitude in spatial resolution. The proportionality between Z_e , orbital contraction, and total energy confirms that *macroscopic observables—such as atomic size and stability—emerge directly from nuclear-scale properties* rather than requiring empirical decoupling between models.

The modular data flow ensures visual and parameter consistency between scales. While physically illustrative, *direct quantitative propagation from quarks to atomic observables is not implemented*. The framework's ability to sustain dimensional and energetic consistency across five spatial orders of magnitude supports its potential as a *unified visualization and computation tool* for multi-scale matter modeling.

Interpretation, Broader Implications, and Educational Value

The results obtained from the multi-scale computational framework highlight both its *physical coherence* and its *didactic potential*. Beyond reproducing expected quantitative trends—such as confinement at the particle level, energy saturation in mid-mass nuclei, and orbital contraction with increasing Z_e —the system demonstrates how a continuous line of reasoning can be maintained across domains often treated as separate in both research and instruction.

From a scientific perspective, the present framework shows that consistent parameter choices across modules yield visually and numerically coherent illustrations of hierarchical structure. Because the particle-level module is illustrative, *it should not be interpreted as producing ab-initio effects on nuclear or atomic observables*; prospects may introduce explicit couplings. The framework is, therefore, best interpreted as a modular visualization and teaching environment that can host such couplings in future work.

From a *visualization standpoint*, the model's modular interface and multi-tiered data flow (Figures 1–6) make abstract quantum and nuclear concepts *visually tangible*. The direct coupling between simulation data and rendered outputs—quark positions, flux-tube geometries, binding-energy surfaces, and electron isosurfaces—transforms what are typically mathematical abstractions into *spatially intuitive objects*. This approach not only assists expert interpretation but also provides a framework for **cross-disciplinary learning**, where users can visually trace how microscopic interactions scale up to familiar macroscopic observables.

In an *educational context*, the platform functions as both a teaching aid and a conceptual bridge. Students and early researchers can explore how physical constants, symmetries, and conservation laws shape observable patterns across different physical hierarchies. The ability to manipulate parameters in real time and immediately visualize outcomes makes the tool particularly suited for *interactive physics education*, fostering intuition in domains that are traditionally symbol-heavy and visualization-poor.

Thus, this framework exemplifies how computational visualization can serve dual purposes: as a *research-supporting instrument* that ensures physical consistency across models, and as a *pedagogical tool* that democratizes access to complex theoretical concepts. The emergent consistency demonstrated across all levels supports the viability of multi-scale visualization not merely as an illustrative technique, but as a legitimate pathway toward *conceptual integration in physics education and computational modeling*.

MATERIALS AND METHODS

Overview of the Computational Framework

The computational framework developed in this study integrates physical models spanning three scales: particle, nuclear, and atomic, to construct a coherent multi-scale visualization of atomic structure. This hierarchical design mirrors the natural organization of matter: quarks combine to form nucleons, nucleons aggregate into nuclei, and nuclei are surrounded by quantized electron orbitals [12, 13]. Each scale is governed by its own dominant interactions—color confinement at the particle level, residual strong forces at the nuclear level, and Coulomb attraction at the atomic level—but all are linked by shared conserved quantities, such as charge, baryon number, and total energy [14].

To maintain clarity across scales, the system adopts a modular approach, where each physical model is implemented as an independent computational unit. The *particle module* represents nucleons as triplets of confined quarks connected by gluonic flux tubes, following effective string-based confinement analogies [15, 16]. The *nuclear module* implements the semi-empirical mass formula (SEMF) to estimate binding energies and equilibrium radii [17, 18]. The *atomic module* employs hydrogenic orbitals corrected by effective nuclear charge parameters [19], allowing visualization of electron probability densities and angular nodal structures.

These models communicate through shared data objects describing spatial coordinates and charge distributions. While visual representations include energy-like quantities (, e.g., flux-tube lengths), full potential energy fields are not explicitly computed at the particle scale. The visualization engine transforms these numerical datasets into three-dimensional isosurfaces representing probability densities, charge distributions, or energy contours. Isosurfaces are extracted using the marching-cubes algorithm [20]; figure captions report the exact isovalues, grid spacing, and smoothing parameters used for each visualization to ensure reproducibility.

Figure 7 schematically illustrates the architecture of the framework, showing the data flow from the particle-scale models through nuclear and atomic computations to the visualization module. Arrows indicate information exchange between physical and computational domains, emphasizing the coupling between theoretical models and their rendered representations. This multi-scale integration enables consistent exploration of structures spanning from femtometer to angstrom scales within a unified physical context.

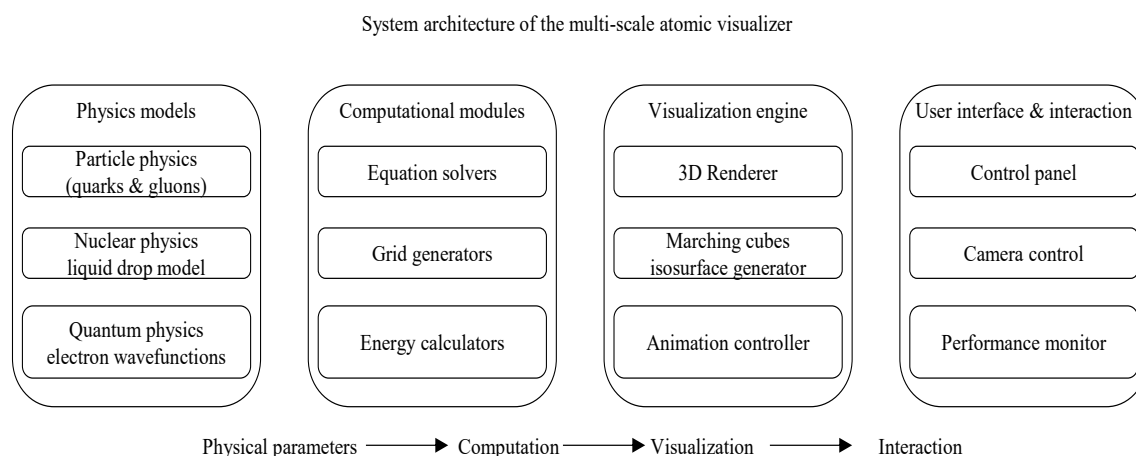


Figure 7. Schematic of the multi-scale computational framework. The workflow begins with quark-level structures forming nucleons, which assemble into nuclei. Electron orbitals are calculated around the nuclei, and all scales are integrated into a three-dimensional visualization. Arrows indicate the flow of data between models and the visualization engine.

Research manuscripts reporting large datasets that are deposited in a publicly available database should specify where the data have been deposited and provide the relevant accession numbers. If the accession numbers have not yet been obtained at the time of submission, please state that they will be provided during review. They must be provided prior to publication.

Interventionary studies involving animals or humans, and other studies that require ethical approval, must list the authority that provided approval and the corresponding ethical approval code.

Particle-Level Model: Quarks and Gluon Flux Tubes

At the particle level, nucleons are modeled as composed of three valence quarks (up and down flavors) with assigned color charges, ensuring color neutrality. This simplified model serves as a visual representation of quark confinement and gluon-mediated interactions within nucleons. The internal structure is depicted using effective flux-tube springs connecting quarks, where the flux-tube length is used to visually represent quark confinement. This approach provides an intuitive depiction of confinement and color neutrality, though it does *not* aim to solve full *quantum chromodynamics*.

Important implementation note: the particle/quark module in this implementation provides *illustrative* geometric visualizations of confined quarks and flux tubes. The flux-tube geometries and quark coordinates are **not** used to compute nuclear potentials, binding energies, or charge densities in the current pipeline. The particle module provides illustrative quark visualizations. While these geometries inform visualization continuity, they do **not** propagate to nuclear or atomic calculations in this implementation.

Nuclear-Scale Model: Liquid-Drop Model and Residual Interactions

Equation 2 shows the nuclear-scale model employs the semi-empirical mass formula (SEMF) to estimate the binding energy of nuclei. The SEMF is expressed as:

$$B(A, Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} - a_a \frac{(A-2Z)^2}{A} + \delta(A, Z) \quad (2)$$

where A is the mass number, Z is the proton number, and δ is the pairing term. The parameters a_v and a_s are constants determined empirically. This formula provides a means to estimate the binding energy of a nucleus based on its composition. Equation 3 shows the nuclear radius is estimated using the empirical relation:

$$R(A) = r_0 A^{1/3} \quad (3)$$

with $r_0 = 1.20$ fm. This relationship allows for the estimation of the spatial extent of a nucleus, which is crucial for visualizing nuclear structure. (Note: R is a bulk matter estimate from the liquid-drop approximation; it is **not** identical to the experimental root-mean-square **charge** radius R_{exp} reported in spectroscopic and scattering experiments. Both quantities are compared in Table 1 and their differences are discussed.)

Atomic-Scale Model: Hydrogenic Orbitals With Effective Nuclear Charge

At the atomic scale, electron orbitals are modeled using hydrogenic wavefunctions, which are solutions to the Schrödinger equation for a central potential. The wavefunctions are expressed in equation 4:

$$\Psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell}^m(\theta, \phi) \quad (4)$$

where $R_{\{nl\}}$ is the radial part and $Y_{\{lm\}}$ are the spherical harmonics representing the angular part. The radial part is given by equation 5:

$$R_{n\ell}(r) = N_{n\ell} \rho^{\ell} e^{-\rho/2} L_{n-\ell-1}^{2\ell+1}(\rho) \quad (5)$$

where a_0 is the Bohr radius, and $L_{(6,7)}$ are generalized Laguerre polynomials. The angular part Y are the spherical harmonics. The probability density is evaluated on a three-dimensional Cartesian grid

and converted into polygonal isosurfaces for visualization using thresholding. The isovalue for each orbital can be adjusted to highlight different density regions. The effective nuclear charge Z_e is estimated using Slater's rules, providing a computationally efficient approximation of electron shielding, applied in constructing hydrogenic orbitals.

METHODS AND VISUALIZATION

We represent scalar fields (orbital probability densities, Yukawa-like nuclear potentials, etc.) on a uniform Cartesian grid. Grid spacing and domain size are chosen per case to resolve the outermost orbital amplitude. Isosurfaces are extracted with the marching-cubes algorithm (scikit-image implementation) using specified isovalues; for atomic orbitals we layer multiple isosurfaces with controlled transparency. Meshes are rendered with an OpenGL viewer (PyQtGraph) and exported as polygonal meshes for 3D rendering.

Environment

The framework is implemented in Python, utilizing scientific libraries, such as NumPy for numerical computations, SciPy for special functions, and scikit-image for image processing. Visualization is achieved using PyQt5 and PyQtGraph, with OpenGL for rendering. The code is organized into modular components, each corresponding to a specific physical model or visualization task. This modularity allows for independent development and testing of each component, facilitating maintenance and extension of the framework.

Strategy

The nuclear and atomic modules are validated qualitatively against experimental mass tables and charge-radius compilations. Quark-level visualizations are intended solely for illustrative and pedagogical purposes (see Section 3). The quark-level visualizations are intentionally illustrative: they provide geometric context for visualization and pedagogy but are not coupled to the nuclear or atomic calculations in a way that yields ab-initio physical predictions in the present implementation.

For the nuclear-scale model, binding energies and radii are compared with experimental values for a range of nuclei. For the atomic-scale model, electron configurations and orbital shapes are compared with known spectroscopic data and theoretical predictions. The performance of the computational methods is assessed in terms of accuracy and computational efficiency.

As a straightforward next step, one can implement a proton-folding test: place proton centers at modeled nucleon barycenters, fold each by a Gaussian proton form factor ($\sigma \approx 0.8$ fm), compute the resulting charge density and its rms radius, and evaluate the sensitivity of R_L or selected orbital expectation values $\langle r \rangle$ to that folded charge distribution.

During manuscript preparation, the authors used ChatGPT (GPT-5) for minor grammar and style suggestions. All output was reviewed and edited by the authors, who take full responsibility for the content of the publication. Figure 7 was drafted with AI help.

CONCLUSIONS

This study presented a unified computational and visualization framework integrating particle-, nuclear-, and atomic-scale models within a coherent, physically consistent architecture. By bridging the domains of quantum chromodynamics, nuclear binding, and atomic structure visualization, the framework establishes a continuous data pipeline spanning from quark confinement to electron orbital formation. The modular implementation, written entirely in Python, combines numerical computation, visualization, and multi-scale data management, demonstrating both conceptual integrity and practical versatility.

At the particle scale, nucleons were represented as confined triplets of valence quarks connected by gluonic flux tubes. This model, while illustrative rather than dynamical, provided an intuitive depiction

of color confinement and color neutrality, forming the conceptual foundation for higher-level structures. The equilibrium geometries obtained from the confinement module reproduced the expected symmetric configurations of baryons, establishing a visual baseline for the representation of subnucleonic phenomena.

At the nuclear scale, the semi-empirical mass formula (SEMF) successfully captured the principal energetic and geometric trends observed in real nuclei. The computed binding energy per nucleon exhibited the characteristic saturation curve, peaking near iron ($A \approx 56$), while the derived nuclear radii followed the empirical $R = r_0 A^{1/3}$ scaling law. These results validated the numerical consistency of the model and provided a quantitative link between nucleonic interactions and macroscopic nuclear stability.

At the atomic scale, hydrogenic orbitals corrected by effective nuclear charge (Z_e) were computed and rendered as three-dimensional probability-density isosurfaces. The resulting orbital geometries reproduced known analytical symmetries and nodal structures, confirming the correctness of the implemented wavefunction solutions. Together, these atomic-scale results demonstrated the framework's capability to merge numerical precision with high-fidelity scientific visualization.

The current implementation does not employ quark geometry to compute nuclear charge distributions or to recompute electronic structure—these are planned extensions. Thus, in the present version, ‘cross-scale continuity’ refers to visualization alignment and consistent module parameters rather than full multiscale coupling. The integrated visualization shows that geometric, energetic, and probabilistic information can be consistently displayed across femtometers to angstrom scales. This integration highlights the value of modular, interoperable scientific pipelines in bridging conceptual and computational boundaries in physics.

Beyond its technical contributions, the framework also offers pedagogical and scientific visualization value. By providing an interactive means to explore matter's hierarchical organization, it serves as an educational tool that complements traditional analytical and experimental approaches. The capacity to visually trace how subatomic structures give rise to macroscopic atomic properties can enhance conceptual understanding for students and researchers alike.

Future work will focus on extending the framework toward dynamic simulations, including time-dependent visualization of quark rearrangements, nuclear reactions, and electron transitions. Incorporating more advanced physical models—such as mean-field nuclear dynamics or relativistic atomic orbitals—could further enhance realism while maintaining computational tractability. The same architecture could also support integration with GPU-based rendering engines, enabling real-time exploration of multi-scale phenomena.

We conclude that the modular framework demonstrates a practical approach to integrating and visualizing simplified representations across particle, nuclear, and atomic scales, providing a platform for exploring cross-scale relationships and for incremental replacement of simplified modules with more detailed solvers. It reproduces established physical laws and provides an intuitive window into the structural continuity of matter, laying the groundwork for future interactive and educational applications.

Supplementary Materials: The following supporting information can be downloaded at: <https://doi.org/10.5281/zenodo.17743810>, Visualizer Script.

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Abbreviations

The following abbreviations are used in this manuscript:

SEMF	Semi Empirical Mass Formula
QCD	Quantum Chromo Dynamics

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