The 30 Most Compelling Pure Thought AI Challenges

A Synthesis Report on Axiom-Driven Scientific Discovery

Synthesized from Domain Expert Analyses

January 12, 2026

Abstract

This report synthesizes analyses across fifteen scientific domains to identify the thirty most compelling challenges that can be tackled using *pure thought and fresh code only*—requiring no external datasets, experiments, or legacy software. Each challenge is grounded in axioms, symmetries, and variational principles, and produces verifiable artifacts: mathematical proofs, certificates, impossibility theorems, or constructive models. These challenges span quantum gravity, materials science, quantum information theory, chemistry, celestial mechanics, and theoretical biology. We outline the mathematical foundations, verification strategies, and expected timelines for each challenge, along with the core computational infrastructure required across all domains.

Contents

1 Introduction

The advent of advanced artificial intelligence systems capable of extended reasoning presents a unique opportunity: the systematic exploration of fundamental scientific questions through *pure thought*. Unlike data-driven or experimental approaches, pure thought challenges rely exclusively on:

- **Axiomatic foundations**: unitarity, causality, crossing symmetry, modular invariance, group theory
- **Mathematical structures**: convex optimization, algebraic topology, representation theory
- **Verifiable artifacts**: machine-checkable proofs, infeasibility certificates, constructive counterexamples
- **Self-written code**: all solvers, verifiers, and proof checkers implemented from first principles

This paradigm eliminates dependence on external datasets, legacy software, or experimental validation, instead producing results whose correctness can be independently verified through mathematical proof.

This report identifies thirty such challenges across six major domains, each selected for:

1. **Scientific impact**: addresses foundational open questions
2. **Tractability**: achievable milestones within 3–12 months
3. **Verifiability**: produces certificates checkable by proof assistants (Lean, Isabelle) or exact solvers
4. **Axiom-driven**: requires no empirical data or experimental inputs

2 Quantum Gravity and Particle Physics

The bootstrap program in quantum field theory and quantum gravity exploits consistency conditions—unitarity, crossing symmetry, causality, and modular invariance—to constrain or uniquely determine physical theories without perturbative expansions[50, 53].

2.1 AdS_3 "Pure Gravity" via the Modular Bootstrap

Challenge: Determine whether extremal two-dimensional conformal field theories (CFTs) with only Virasoro descendants below the gap exist for large central charge $c = 24k$, corresponding to pure AdS_3 gravity duals.

Why Compelling: The existence or rigorous impossibility of such theories would resolve a foundational question in the AdS/CFT correspondence[21, 36]. Extremal CFTs at $c = 24$ are related to the Monster group, and their generalization to $c = 24k$ remains open.

Pure Thought Approach:

- Implement high-precision modular bootstrap solvers combining linear programming (LP) and semidefinite programming (SDP) with exact rational certificates
- Enforce modular invariance: $\mathcal{Z}(\tau) = \mathcal{Z}(-1/\tau)$, unitarity (positive degeneracies), and integrality constraints

- Search for feasible partition functions with specified spectral gaps
- When infeasible, extract dual certificates proving impossibility for given (c, Δ_{gap}) pairs

Verifiable Artifacts: SDP dual functionals (exact rational certificates), infeasibility proofs, or explicit extremal spectra

Timeline: 60–90 days to reproduce known constraints (e.g., $k = 1$ Monster point); 6–12 months for new results

2.2 Gravitational Positivity and Causality Bounds

Challenge: Derive rigorous bounds on higher-derivative operators (e.g., R^2, R^3 terms) in graviton effective field theories using analyticity, crossing, unitarity, and causality constraints.

Why Compelling: Determines which low-energy effective theories are UV-completable into consistent quantum gravity theories—central to the "swampland" program[46, 61]. Gravitational causality imposes stringent constraints through shockwave/eikonal scattering[10].

Pure Thought Approach:

- Implement dispersion relations with subtractions compatible with massless graviton poles
- Handle t-channel singularities and Regge growth rigorously
- Formulate as convex optimization problems (Sum-of-Squares, SDP)
- Output dual certificates (polynomials or SOS decompositions) proving regions are forbidden/allowed

Verifiable Artifacts: Multi-coupling bounds with machine-checkable proofs; dual polynomial certificates

Timeline: 3–9 months

2.3 Celestial CFT Bootstrap

Challenge: Carve out the consistent space of celestial CFTs by enforcing $\mathrm{SL}(2, \mathbb{C})$ covariance, crossing symmetry, unitarity, and soft-theorem constraints on celestial correlators for graviton scattering.

Why Compelling: Connects four-dimensional quantum gravity to two-dimensional celestial CFT structure—a new holographic paradigm[47, 52].

Pure Thought Approach:

- Develop Mellin transform pipeline for tree and one-loop amplitudes derived from first principles
- Impose celestial crossing equations, Regge bounds, and soft limits (Weinberg's soft graviton theorem[63]) as SDP inequalities
- Produce extremal functionals certifying or excluding OPE data patterns

Verifiable Artifacts: Rigorous "islands" or no-go regions for subsectors

Timeline: 6–12 months

2.4 Modular-Lightcone Bootstrap for Holographic CFTs

Challenge: For large central charge c, sparse-spectrum CFTs (holographic theories), derive sharp bounds on higher-spin gaps and OPE coefficients implied by causality/chaos constraints and crossing symmetry.

Why Compelling: Provides quantitative "gravitational bootstrap" constraints[34]—rules out bulk higher-derivative terms that would violate causality or the chaos bound.

Pure Thought Approach:

- Implement Lorentzian inversion formula[12] and lightcone expansions
- Certify inequalities via SDP/SoS, producing formal certificates
- Prove that certain bulk operators must be small or vanish to avoid superluminality or averaged null energy condition (ANEC) violations

Verifiable Artifacts: Tighter exclusion plots for higher-spin exchanges with dual certificates
Timeline: 6–9 months

2.5 Positive Geometry for Gravity

Challenge: Identify or rule out amplituhedron-like positive-geometry structures[2] for (super)gravity sectors beyond planar $\mathcal{N} = 4$ super-Yang–Mills.

Why Compelling: Would reveal hidden mathematical structures in quantum gravity amplitudes or prove fundamental obstructions to such structures existing in gravity theories.

Pure Thought Approach:

- Implement canonical-form solvers for polytopes and Grassmannians
- Use finite-field sampling plus rational reconstruction for loop integrands
- Verify symbol integrability and coproduct consistency
- Search for minimal geometries reproducing graviton integrands from on-shell recursion and unitarity cuts

Verifiable Artifacts: New positive-geometry proposals or no-go theorems for specific helicity/loop sectors

Timeline: 9–12 months

2.6 Non-perturbative S-matrix Bootstrap with Gravity

Challenge: Carve out the space of unitary, crossing-symmetric, analytic $2 \to 2$ amplitudes obeying gravitational soft theorems and proper high-energy behavior.

Why Compelling: First rigorous non-perturbative constraints on quantum gravity coupled to matter[48].

Pure Thought Approach:

- Build partial-wave and Roy-like equation machinery adapted to massless exchange
- Impose Weinberg soft behavior as hard constraints
- Solve as convex feasibility problem; return dual certificates excluding inconsistent Wilson-coefficient tuples

Verifiable Artifacts: Dual certificates; islands and exclusion regions in parameter space
Timeline: 6–12 months

2.7 Extremal Higher-Dimensional CFTs with Stress Tensor

Challenge: Determine whether "nearly extremal" unitary CFTs exist in $d = 3, 4$ dimensions with large gaps to higher-spin currents, corresponding to pure Einstein gravity in AdS.

Why Compelling: Connects CFT bootstrap constraints to the existence and uniqueness of pure gravity in AdS[23].

Pure Thought Approach:

- Mixed-correlator bootstrap including stress tensor $T_{\mu\nu}$
- Use extremal functional method[17] to certify islands or no-go results via dual functionals

Verifiable Artifacts: Stronger universal lower bounds on higher-spin gaps
Timeline: 6–12 months

2.8 Swampland via Modularity and Higher-Form Symmetries

Challenge: Use modularity, integrality, and higher-form symmetry constraints to produce theorem-level obstructions to quantum-gravity-inconsistent spectra.

Why Compelling: Mathematically rigorous "no-go" theorems for theories in the swampland[61]—identifies which quantum field theories cannot be UV-completed to gravity.

Pure Thought Approach:

- Couple modular bootstrap to discrete/higher-form anomaly constraints (cobordism approach[38])
- Generate infeasibility certificates for partition functions/OPE data subject to symmetry charges

Verifiable Artifacts: "No such CFT" results under explicit symmetry assumptions
Timeline: 9–12 months

3 Materials Science

Modern materials theory increasingly relies on symmetry principles and topological invariants, enabling predictions from group theory and K-theory without materials-specific parameters[6, 62].

3.1 Topological Band Theory Without Materials Data

Challenge: Complete constructive classification of which band topologies are possible for minimal orbital contents and symmetries across all (magnetic) space groups, plus minimal tight-binding models realizing them.

Why Compelling: Foundational atlas mapping symmetry → achievable topologies with rigorous theorems and no-go results[49].

Pure Thought Approach:

- Compute elementary band representations (eBRs) for all Wyckoff positions[11]
- Enumerate minimal tight-binding graphs per space group
- Certify Chern and $\mathbb{Z}_2$ invariants via K-theory and Wilson loops

- Prove nodal features enforced by nonsymmorphic symmetries

Verifiable Artifacts: Atlas of minimal models with proofs; no-go theorems where impossible
Timeline: 3–6 months (non-magnetic); 6–12 months (magnetic groups)

3.2 Flat Chern Bands with Provable Geometry

Challenge: Design compact tight-binding lattices realizing flat bands with target Chern numbers and provably optimal quantum geometry (uniform Berry curvature, optimal Fubini–Study metric bounds).

Why Compelling: Critical for fractional Chern insulator realization[44]—provides blueprints with mathematical guarantees for fractionalization.

Pure Thought Approach:

- Enumerate finite-range hopping graphs
- Certify Chern numbers exactly via lattice index theorems
- Prove lower bounds on flatness ratio using Sum-of-Squares (SoS) relaxations
- Generate Wannier obstruction certificates as topological proofs

Verifiable Artifacts: Hamiltonians with certificates of Chern number, flatness bounds, and Wannier obstruction

Timeline: 6–9 months

3.3 RBCE: Relativistic Band and Crystal-Field Engineering

Challenge: Proof-level classification of single-ion anisotropy and g-tensor anisotropy for all d^n configurations across every point group, identifying maximizers of magnetocrystalline anisotropy.

Why Compelling: Enables "rare-earth-like behavior without rare earths"—critical for permanent magnets and quantum materials[42]. Spin-orbit coupling (SOC) in $4d/5d$ systems can mimic lanthanide anisotropy.

Pure Thought Approach:

- Enumerate point-group irreducible representations (irreps)
- Build crystal-field plus SOC Hamiltonians symbolically
- Derive closed-form anisotropy energy expansions
- Prove upper bounds on K_1, K_2 versus CF/SOC parameters for each symmetry
- Determine necessary/sufficient symmetry conditions for Ising-like single-ion behavior

Verifiable Artifacts: Theorem-backed atlas: (site symmetry, d^n) $\rightarrow$ allowed splitting patterns, max-anisotropy certificates, explicit model Hamiltonians

Timeline: 6–12 months

3.4 Photonic/Phononic Crystals: Rigorous Bandgap Optimization

Challenge: Design microstructures (2D/3D) with certified complete bandgaps at lowest possible index contrast, with provable gap-to-midgap maxima under symmetry and fill-fraction constraints.

Why Compelling: Yields fabrication-ready unit cells with airtight mathematical guarantees[35].

Pure Thought Approach:

- Build verified FEM/plane-wave eigensolvers with interval arithmetic
- Output rigorous lower/upper eigenvalue bounds $\Rightarrow$ certified gap
- Conduct topology optimization under symmetry groups
- Prove optimality via dual (SoS/shape-derivative) certificates or constructive near-optima with *a posteriori* bounds

Verifiable Artifacts: Microstructure blueprints plus interval-verified band diagrams and dual certificates

Timeline: 6–9 months

3.5 Universal Bounds for Effective Properties of Composites

Challenge: Derive sharp bounds on effective conductivity, permittivity, and elasticity for given phase properties, volume fractions, and symmetries; cross-property bounds linking elastic and thermal responses.

Why Compelling: Goes beyond classical Hashin–Shtrikman bounds[22]—fundamental limits no microstructure can beat.

Pure Thought Approach:

- Formulate G-closure problems[39] as SDP moment relaxations
- Produce exact dual certificates giving provable bounds
- Construct microstructures attaining bounds via algorithmic inverse homogenization
- Verify with interval-certified solvers

Verifiable Artifacts: New analytical bounds, constructive microstructures, proof certificates

Timeline: 9–12 months

3.6 Topological Mechanics: Maxwell Frames and Programmable Metamaterials

Challenge: Complete classification and constructive design of Maxwell frames with topological polarization (robust boundary modes) and programmable mechanical response.

Why Compelling: Bridges rigidity theory and topological physics[27]—enables mechanical metamaterials with guaranteed properties.

Pure Thought Approach:

- Enumerate periodic frameworks under space-group constraints
- Compute topological invariants (e.g., winding of $\det R(\mathbf{k})$)
- Use SAT/MILP to enforce isostaticity, target mode counts, forbidden self-stresses

- Certify with DRAT proofs and symbolic checks

Verifiable Artifacts: Lattice designs with certified zero-mode counts and topological indices; printable unit cells

Timeline: 6–9 months

3.7 Real-Space Topological Invariants for Disordered Media

Challenge: Certified algorithms for Chern/$\mathbb{Z}_2$ indices in aperiodic/disordered systems with finite-volume error bounds.

Why Compelling: Extends topological classification beyond perfect crystals using noncommutative geometry[3, 51].

Pure Thought Approach:

- Implement noncommutative Chern numbers, Bott indices, spectral localizers
- Prove *a priori* error bounds versus system size and disorder strength
- Provide interval-verified invariants for generated disordered samples

Verifiable Artifacts: Algorithms with proofs; reference models showing certified quantization in finite domains

Timeline: 9–12 months

4 Chemistry

Quantum chemistry from first principles uses variational principles and convexity, enabling bounds and constraints without empirical fitting[33].

4.1 N-Representability and 2-RDM Variational Chemistry

Challenge: Close the gap between necessary and sufficient constraints for two-electron reduced density matrix (2-RDM) feasibility; deliver provably tighter constraint families.

Why Compelling: Direct path to ground-state energies without computing the wavefunction[37]—foundationa for quantum chemistry.

Pure Thought Approach:

- Pure convex geometry: energies are linear in the 2-RDM
- Implement 2-RDM SDP solver with exact rational logging
- Add hierarchies beyond P, Q, G, T constraints via moment/SOS relaxations with symmetry reduction
- Prove constraint validity in classes: pairing Hamiltonians, 1D fermions, Hubbard-like models

Verifiable Artifacts: Ground-state lower bounds with SDP dual certificates; infeasibility certificates; Lean-formalized lemmas

Timeline: 6–9 months

4.2 Non-empirical Density Functional Theory via Convex Analysis

Challenge: Characterize the cone of exchange-correlation (XC) functionals satisfying all exact constraints (scaling, spin bounds, Lieb–Oxford[32], Lieb convexity); construct extremal functionals.

Why Compelling: DFT from first principles—no empirical fitting, only mathematical constraints.

Pure Thought Approach:

- Encode constraints as convex sets
- Use support-function computations (SDP/SoS) to produce functionals and guaranteed energy bounds
- Build self-interaction-free subclass; prove tightness on canonical test densities

Verifiable Artifacts: Certified XC bounds with proofs of constraint satisfaction; analytic forms or numeric oracles

Timeline: 9–12 months

4.3 Strictly-Correlated Electrons as Multi-Marginal Optimal Transport

Challenge: Compute and bound the SCE functional $W_{\mathrm{SCE}}[\rho]$ by solving multi-marginal optimal transport with Coulomb cost; derive co-motion function constructions.

Why Compelling: Pure optimal transport formulation of strong-correlation limit[20, 55]—mathematically elegant and rigorous.

Pure Thought Approach:

- Sparse/discretized OT with exact certificates (duality gaps $\Rightarrow$ provable bounds)
- Symmetry-adapted decompositions for spherical and crystalline densities

Verifiable Artifacts: Certified upper/lower bounds on W_{SCE} with dual potentials as proof objects

Timeline: 9–12 months

4.4 Complete Isomer Enumeration with Proofs

Challenge: Exhaustively enumerate constitutional and stereoisomers up to size N under valence rules, with isomorphism certificates proving completeness.

Why Compelling: Resolves fundamental combinatorial questions in chemical space[18].

Pure Thought Approach:

- Pólya–Redfield enumeration plus canonical labeling
- SAT to enforce stereochemical constraints
- Emit DRAT proofs of completeness and minimality

Verifiable Artifacts: Exact counts, canonical SMILES/graphs, proof logs

Timeline: 6–9 months

4.5 Inverse Statistical Mechanics: Potentials with Provable Ground States

Challenge: Design pair or few-body potentials that provably stabilize target crystals (diamond, wurtzite, bcc) over ranges of densities and temperatures.

Why Compelling: "Potentials with proofs"[58]—enables rational design of self-assembling materials with mathematical guarantees.

Pure Thought Approach:

- Extend Cohn–Kumar sphere-packing bounds[15] to 3D molecular settings
- Compute rigorous energy gaps with interval-verified lattice sums (Ewald summation)

Verifiable Artifacts: Closed-form potentials plus proofs of stability; parameter maps with certified gaps

Timeline: 6–12 months

5 Quantum Information and Many-Body Theory

Quantum information theory provides operational characterizations of resources (entanglement, magic, coherence) through convex cones and certification hierarchies[26].

5.1 LDPC and Hypergraph-Product Quantum Error Correcting Codes

Challenge: Construct new QECC families with better rate–distance–degree tradeoffs and provable decoding guarantees in adversarial/noise-model-free regimes.

Why Compelling: Critical for scalable quantum computing[7, 57]—approaching capacity with practical constraints.

Pure Thought Approach:

- Pure combinatorics and algebraic topology
- LLM-led search over Tanner graphs and topological constructions
- SAT for distance certificates (lower bounds via integer programming)
- Design BP/OSD/ML decoders with provable worst-case bounds

Verifiable Artifacts: Code constructions with distance/minimum-weight certificates (SAT/ILP proofs); impossibility theorems for certain parameter triples

Timeline: 90 days to novel instances; 12 months for infinite families with improved asymptotics

5.2 New Bell Inequalities and Tsirelson-type Bounds

Challenge: Discover Bell inequalities with maximal quantum–classical gaps; certify with Navascués–Pironio–Acín (NPA) duals[41].

Why Compelling: Fundamental tests of quantum nonlocality with tight bounds—deepens understanding of the quantum–classical boundary.

Pure Thought Approach:

- Noncommutative SDP/SoS for operator inequalities
- Auto-search inequality families

- Produce SDP dual certificates proving optimality of quantum values

Verifiable Artifacts: Inequality families with optimal quantum values (SDP duals) and explicit achieving measurements/states

Timeline: 6–9 months

5.3 Certified Spectral Gaps for Parent Hamiltonians

Challenge: Generalize Knabe/martingale techniques[29] to automate discovery of local gap witnesses for MPS/PEPS parent Hamiltonians.

Why Compelling: Rigorous many-body theory—provable lower bounds on gaps guarantee phases of matter.

Pure Thought Approach:

- Tensor-network engine with interval arithmetic error bars
- Automated gap-witness search producing machine-checked inequalities
- Parent Hamiltonian construction and verification

Verifiable Artifacts: Provable lower bounds on gaps for new MPS/PEPS families; Lean/Isabelle lemmas

Timeline: 6–12 months

5.4 Topological Order and Anyon Condensation with Proofs

Challenge: Classify gapped boundaries and defects; derive anomaly constraints on 2D/3D topological orders from categorical data.

Why Compelling: Complete mathematical understanding of topological phases[28]—fusion rules, braiding, and anomalies.

Pure Thought Approach:

- Fusion categories and modular tensor category (MTC) data
- Anomaly tests via obstruction cocycles with machine-checked coherence
- Construct exactly-solvable commuting-projector models (e.g., string-net models[31])

Verifiable Artifacts: Fusion/braiding tables with obstruction cocycle certificates; explicit Hamiltonians

Timeline: 9–12 months

5.5 Sign-Problem (Un)avoidability

Challenge: Decide stoquasticity under local basis changes; characterize classes where sign-free forms are impossible.

Why Compelling: Resolves fundamental question about quantum Monte Carlo applicability[59]—sharp dividing line between tractable and intractable problems.

Pure Thought Approach:

- SAT/ILP encodings to search for basis transformations making Hamiltonian stoquastic
- Certificates of (non)existence

- Explicit unitaries achieving sign-free form when possible

Verifiable Artifacts: Certificates of stoquasticity or impossibility proofs; explicit basis transformations

Timeline: 6–9 months

6 Planetary Systems and Celestial Mechanics

Classical celestial mechanics provides ideal testing grounds for computer-assisted proofs of long-time stability and rigorous dynamics[13].

6.1 KAM/Nekhoroshev Stability Domains for Planetary Systems

Challenge: Compute quantitative Kolmogorov–Arnold–Moser (KAM) existence and Nekhoroshev stability domains for near-integrable multi-planet Hamiltonians, including post-Newtonian corrections.

Why Compelling: Rigorous long-time stability guarantees for planetary systems[1, 43]—pure dynamical systems theory with explicit time-scale bounds.

Pure Thought Approach:

- High-order averaging (Lie transforms, Birkhoff normal forms) with validated numerics
- Bound remainders rigorously; compute Diophantine constants
- Certify invariant tori existence and long-time action confinement

Verifiable Artifacts: Formal normal forms plus interval certificates for tori existence and explicit exponential time-scale bounds

Timeline: 9–12 months

6.2 Periodic Orbits and Invariant Manifolds in N-Body Problem

Challenge: Discover new families of periodic orbits in N-body and restricted three-body problems; classify stability via validated Floquet analysis.

Why Compelling: Fundamental objects in celestial mechanics[14]—"choreographies" and transport structures with machine-verified existence.

Pure Thought Approach:

- Variational solvers with symmetry constraints
- Validated continuation (Krawczyk operator, radii polynomials[60]) to enclose true orbits and multipliers
- Conley index and covering relations[64] for heteroclinic connections

Verifiable Artifacts: Libraries of orbits with machine-verified existence/stability; connection proofs with interval error bounds

Timeline: 6–9 months

6.3 Central Configurations Classification

Challenge: Certified classification of central configurations for $N = 5$–8 under symmetry and mass patterns; prove upper/lower bounds on their counts.

Why Compelling: Classic Smale problem[56]—polynomial systems amenable to complete algebraic certification.

Pure Thought Approach:

- Gröbner basis and resultant elimination
- α-theory (Smale's α-theory[5]) to certify isolated solutions
- SAT proofs for nonexistence in constrained subcases

Verifiable Artifacts: Exhaustive catalogs with proof certificates
Timeline: 6–12 months

7 Biology and Origin of Life

Theoretical biology increasingly uses information theory, dynamical systems, and combinatorics to establish fundamental limits[54].

7.1 Minimal Autocatalytic Cores and Universality

Challenge: Find provably minimal chemical reaction networks (CRNs) that are autocatalytic or universal (can implement arbitrary computation/self-replication) under mass-action kinetics.

Why Compelling: Foundational for origin-of-life theory[25]—what is the simplest chemistry capable of self-replication?

Pure Thought Approach:

- CRNs are finite algebraic objects; properties reduce to graph/semigroup and dynamical criteria
- Compute stoichiometric kernels, siphons/traps, deficiency/endotacticity tests[19]
- Branch-and-bound with isomorphism-free enumeration
- DRAT/SMT certificates of minimality and infeasibility

Verifiable Artifacts: Catalog of minimal autocatalytic sets with machine-checkable witnesses; Lean proofs for key lemmas
Timeline: 6–9 months

7.2 Genotype→Phenotype Channel Capacity Bounds

Challenge: Derive upper/lower bounds on mutual information between genome of length L and coarse-grained phenotype under biophysically constrained maps.

Why Compelling: Fundamental limits on biological design[4]—what information can evolution actually encode?

Pure Thought Approach:

- Model genotype→phenotype as constrained circuits or graph dynamics

- Derive rate–distortion and Fano/Le Cam lower bounds
- Construct achievability codes (explicit mappings) to close gaps

Verifiable Artifacts: Theorems with constructive encoders/decoders and proofs of capacity bounds

Timeline: 9–12 months

8 Core Infrastructure: The Day-0 Toolchain

All thirty challenges share common computational and proof infrastructure that should be built once and reused across domains.

8.1 Autoprover Farm

Purpose: Multi-agent proof workshop that proposes lemmas, attempts multiple proof styles (induction, contradiction, sum-of-squares, compactness), and interfaces with proof assistants.

Components:

- Lean 4[16] and Isabelle/HOL[45] integration
- Automated theorem discovery and lemma generation
- Proof strategy search (enumeration, refinement, analogy)
- Human-readable proof synthesis from machine certificates

8.2 Symbolic-Numeric Engine

Purpose: From-scratch computer algebra system with exact arithmetic and certified numerics.

Components:

- Exact rational and algebraic number arithmetic
- Gröbner basis computation[9] and resultants
- Interval arithmetic[40] and Taylor models
- Automatic differentiation
- Self-implemented SDP/LP/QP solvers with dual certificate logging
- Sum-of-Squares (SoS) hierarchy implementation[30]

8.3 Search with Certificates

Purpose: Combinatorial search algorithms that produce machine-checkable proof logs.

Components:

- SAT solvers (CDCL) with DRAT/FRAT proof logging[24]
- SMT solvers (DPLL(T)) with proof generation
- Branch-and-bound for optimization with cutting-plane proofs
- A^* and constraint propagation over combinatorial spaces

8.4 Bootstrap and Amplitude Toolbox

Purpose: Specialized tools for conformal bootstrap and scattering amplitude calculations.
Components:

- Conformal block computation (recursion relations, differential equations)
- Crossing equation setup and SDP formulation
- Symbol alphabet computation and integrability checks
- Finite-field sampling and rational reconstruction
- IBP (integration-by-parts) reduction algorithms
- On-shell recursion (BCFW[8]) and generalized unitarity

8.5 Tensor Network and Coding Theory Lab

Purpose: Tensor network algorithms and quantum/classical code construction.
Components:

- MPS/PEPS/MERA contraction algorithms with rigorous error bars
- Variational optimization for ground states
- Parent Hamiltonian construction
- Stabilizer code manipulation and distance computation
- Classical/quantum LDPC code construction
- Decoding algorithm implementation and analysis

8.6 Proof Back-Ends

Purpose: Export all results to independently verifiable formats.
Formats:

- Lean/Isabelle theorem statements and proofs
- DRAT/FRAT unsatisfiability proofs for SAT
- SDP dual certificates (exact rational matrices)
- Interval arithmetic enclosures with guaranteed error bounds
- Gröbner basis ideal membership certificates

9 Selection Principles and Execution Strategy

9.1 Why These 30 Challenges?

Each challenge was selected based on five criteria:

1. **Proofs over predictions**: Resolves to theorems, bounds, constructive counterexamples, or certificates—not approximate numerics
2. **Axiom-driven**: Relies exclusively on unitarity, causality, crossing, locality, symmetry, convexity (physics); quantum mechanics and variational principles (chemistry); formal axioms (mathematics/computer science)
3. **Verifiable search**: Uses massive search guided by reasoning systems, but demands fast verifiers (proof checkers, symbolic algebra, certificate validation)
4. **Formalized by default**: Produces both human-readable proofs and machine-checkable artifacts (Lean/Isabelle, DRAT/FRAT, SoS certificates, interval bounds)
5. **Tractable with impact**: Achievable milestones within 3–12 months addressing foundational open questions

9.2 Execution Pattern

For each track:

1. **Toolchain development**: Emit self-contained solver + checker + proof exporter
2. **Many-shot strategy generation**: Vary gauges, bases, relaxations, search strategies
3. **Parallel search with early certification**: Run multiple proof attempts in parallel; immediately verify candidates
4. **Human-readable synthesis**: Once machine certificate exists, synthesize polished exposition

9.3 Resource Allocation

Token/compute budget:

- 80% to search and proof attempts
- 20% to verification and proof polishing

Initial focus (highest-likelihood short-term wins):

1. AdS_3 modular bootstrap (Track 1)
2. LDPC quantum codes (Track 21)
3. Minimal autocatalytic networks (Track 29)
4. RBCE symmetry atlas (Track 11)
5. Gravitational positivity bounds (Track 2)

9.4 12-Month Roadmap

Months 1–2: Stand up core infrastructure

- Autoprover Farm with Lean/Isabelle integration
- Symbolic-Numeric Engine with interval arithmetic
- SAT/SMT with proof logging
- SDP/SoS solver with exact certificates

Months 3–4: Validate pipelines

- Reproduce cornerstone results in bootstrap, integrals, Ramsey numbers
- Verify certificate formats and proof assistant integration

Months 5–8: Push new bounds

- New bootstrap bounds (Tracks 1, 4)
- First novel QECC families (Track 21)
- RBCE anisotropy atlas (Track 11)
- Gravitational causality bounds (Track 2)

Months 9–12: Deliver results

- At least 3 "best-known" results with machine-checkable proofs
- One structural classification (Track 9 or 11)
- Publication-ready manuscripts with proof repositories

10 Conclusion

This portfolio of thirty pure thought challenges represents the frontier of what mathematical reasoning, amplified by advanced artificial intelligence, can achieve in fundamental science. Unlike data-driven or experimental approaches, these challenges require:

- **No external datasets**: all information derives from axioms and first principles
- **No experiments**: verification is mathematical, not empirical
- **No legacy software**: all solvers implemented from scratch with proof generation

The results—theorem-level bounds, impossibility certificates, constructive models—are independently verifiable through proof assistants and exact arithmetic, ensuring correctness without trust.

Success across even a subset of these challenges would demonstrate that pure mathematical reasoning, when properly formalized and computationally amplified, can resolve longstanding open questions spanning quantum gravity, materials design, quantum information, chemistry, celestial mechanics, and theoretical biology.

The key innovation is not numerical approximation but *certified reasoning*: every claim accompanied by a machine-checkable proof. This paradigm complements experimental and computational science with a third pillar—*axiomatic science*—where progress is measured not in predictive accuracy but in theorems proven.

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