

Agentic AI-Driven Negative Emission Optimization: Large Language Model Orchestration and Quantum Annealing for Real-Time Carbon Capture Policy Simulation Beyond 1.5°C Thresholds

Mayuresh Sharma^{1*}, Aryan Sinha²

Abstract

The convergence of agentic artificial intelligence, large language model (LLM) orchestration, and quantum annealing presents a transformative paradigm for climate policy computation. This paper introduces Nega Optima a multi-agent computational architecture that integrates LLM-driven policy parsing, quantum annealing-based combinatorial optimization, and real-time integrated assessment model (IAM) feedback loops to simulate negative emission technology (NET) deployment strategies in a post-1.5°C overshoot scenario. Existing carbon capture optimization frameworks suffer from three systemic limitations: static policy inputs, classical solver intractability at continental deployment scales, and the absence of closed-loop policy refinement mechanisms. Nega Optima addresses these gaps through a hierarchical agent topology in which a Coordinator LLM agent decomposes multi-decadal climate targets into callable subtasks, delegating combinatorial fleet allocation problems to a hybrid quantum-classical annealer built on D-Wave Advantage architecture, while simultaneously streaming scenario outputs back to a Critic LLM agent for policy-coherence verification. Experimental results across 1,200 policy scenario simulations demonstrate that Nega Optima achieves a mean time-to-optimal-solution reduction of 67.3% relative to MILP baselines, with a carbon capture portfolio deviation of less than 4.2% from IPCC AR6 CDR pathway benchmarks. The framework further demonstrates robust equity-aware allocation under Land Use, Land-Use Change, and Forestry (LULUCF) constraints, reducing land competition conflicts by 41% in South and Southeast Asian deployment scenarios. These findings establish Nega Optima as a computationally credible and policy-relevant instrument for navigating the carbon budget emergency. (1) Nega Optima: first agentic AI framework coupling LLM orchestration with quantum annealing for NET policy optimization. (2) 67.3% reduction in solve time vs. classical MILP solvers across 1,200 scenario benchmarks. (3) Closed-loop Critic-LLM mechanism enforces policy coherence and UNFCCC alignment in real time. (4) Equity-weighted LULUCF constraints reduce land-conflict index by 41% in Asia-Pacific scenarios. (5) CDR portfolio deviation <4.2% from IPCC AR6 C1–C3 pathways under Monte Carlo uncertainty.

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INTRODUCTION

The trajectory of anthropogenic greenhouse gas emissions has rendered the 1.5°C Paris Agreement target increasingly precarious [1-3]. The Intergovernmental Panel on Climate Change Sixth

Assessment Report (IPCC AR6, [4]2022) projects that in all scenarios limiting warming to $\leq 1.5^{\circ}\text{C}$ with limited or no overshoot, carbon dioxide removal (CDR) must remove between 100 and 1,000 GtCO₂ cumulatively by 2100. This represents not merely a technical challenge but a decision-theoretic problem of extraordinary dimensionality: the selection, timing, scale, geographic distribution, and co-benefit tradeoffs of negative emission technologies (NETs) such as Bioenergy with Carbon Capture and Storage (BECCS), Direct Air Carbon Capture and Storage (DACCS), enhanced weathering, and afforestation/reforestation cannot be optimally resolved by conventional sequential policy analysis [2].

Contemporary approaches to CDR portfolio optimization exhibit three structural deficiencies. First, static integrated assessment models (IAMs) such as GCAM, MESSAGE-GLOBIOM, and REMIND operate on decadal timesteps with pre-specified scenario pathways, precluding the real-time responsiveness that dynamic policy environments demand. Second, the combinatorial nature of multi-region, multi-technology NET deployment renders classical Mixed-Integer Linear Programming (MILP) approaches computationally intractable beyond approximately 500 decision variables a scale far smaller than continental deployment realities. Third, the translation of unstructured policy text (legislation, UNFCCC nationally determined contributions, carbon pricing schemes) into computable parameters remains a manual, error-prone bottleneck that introduces systemic latency into the policy cycle [3].

Recent advances in three distinct computational domains present an opportunity to address these limitations simultaneously. Agentic large language model frameworks exemplified by architectures such as React, AutoGen, and Lang Graph enable autonomous multi-step reasoning, tool invocation, and iterative self-critique, making them well-suited to the orchestration of complex, multi-stage computational pipelines. Quantum annealing, particularly the D-Wave Advantage system with over 5,000 physical qubits and Pegasus topology connectivity, offers a physically grounded heuristic for finding near-ground-state solutions to Quadratic Unconstrained Binary Optimization (QUBO) problems the canonical form into which many combinatorial optimization problems can be mapped. Hybrid quantum-classical solvers further extend this capability to larger, constrained problems through decomposition strategies such as Quantum Branch-and-Bound (QBB) and Tabu-augmented annealing [4].

This paper presents Nega Optima, a novel agentic AI framework that systematically integrates these three capabilities into a coherent, deployable system. The primary contributions of this work are:

1. A formal specification of the Nega Optima multi-agent architecture including Coordinator, Optimizer, IAM-Interface, and Critic agent roles.
2. A QUBO formulation of the NET fleet allocation problem incorporating equity-weighted land-use constraints.
3. Empirical benchmarking against MILP and simulated annealing baselines across 1,200 IPCC-aligned scenario simulations.
4. A qualitative analysis of policy coherence enforcement via LLM-driven Critic feedback under UNFCCC compliance criteria.

BACKGROUND AND RELATED WORK

Negative Emission Technologies and the CDR Imperative

CDR technologies span a spectrum from nature-based solutions (afforestation, soil carbon sequestration, blue carbon) to engineered systems (DACCS, BECCS, ocean alkalinity enhancement). BECCS, which combines bioenergy production with geological carbon storage, has historically dominated IAM pathways due to its dual energy-carbon benefit. However, BECCS deployment at the scale required potentially 3–10 GtCO₂/yr by 2050 faces severe land-use competition, water stress, and biodiversity trade-offs that have led to widespread criticism of IAM over-reliance on this single technology. DACCS, by contrast, is land-efficient but currently operates at a levelized cost of approximately USD 300–600/tCO₂, limiting near-term scalability. A diversified CDR portfolio is therefore a climate-policy imperative, not merely a technical preference [5].

Optimization Approaches for Carbon Policy

The application of operations research to climate policy dates to the 1970s, but its computational relevance has expanded dramatically with the emergence of high-resolution energy system models. Capacity expansion models such as OSeMOSYS and TIMES employ LP/MILP formulations to minimize system cost subject to energy balance, emissions, and technology constraints. More recent work by Luderer et al. [7] (2021) and Bauer et al. [6] (2017) has explored stochastic programming and robust optimization approaches to account for technology cost uncertainty. However, none of these frameworks incorporate real-time LLM-mediated policy parsing or quantum-enhanced solvers the key innovation space Nega Optima occupies [8-14].

Quantum Annealing for Combinatorial Optimization

Quantum annealing exploits quantum tunneling to escape local minima in energy landscapes defined by Ising Hamiltonians. D-Wave's physical annealing approach maps optimization problems onto the hardware's qubit connectivity graph, solving QUBO instances of the form: minimize $x^T Q x$, where $x \in \{0,1\}^n$ and Q is an upper-triangular matrix of real-valued coefficients. Recent comparative studies (McGeoch & Wang, [8] 2023; Yarkoni et al., [15] 2022) demonstrate quantum speedup for specific problem classes particularly sparse, frustrated graph problems though generalizable quantum advantage for industrial-scale optimization remains an active research frontier. Hybrid solvers that partition large QUBOs into sub-problems compatible with hardware qubit counts have demonstrated practical speedups for vehicle routing, financial portfolio optimization, and logistics scheduling [9].

Agentic LLM Architectures

The agentic AI paradigm extends LLMs from passive response generators to active, goal-directed agents capable of planning, tool use, self-correction, and multi-agent collaboration. The React framework (Yao et al., [14] 2023) formalized the interleaving of reasoning and action traces within a single LLM context. AutoGen (Wu et al., [13] 2023) introduced structured conversation protocols between specialized LLM agents, enabling modular workflows where agents take on roles such as planner, executor, and reviewer. Lang Graph extends this to stateful, cyclic computational graphs with explicit state machines. Despite rapid growth in applications including scientific literature review, drug discovery, and software engineering no prior work has applied agentic LLM architectures to climate policy simulation or quantum optimization orchestration [10].

SYSTEM ARCHITECTURE: NEGA OPTIMA

Architectural Overview

Nega Optima is organized as a directed computational graph with four specialized LLM agents and one quantum-classical solver subsystem, The agent roles are:

- *Coordinator Agent*: A GPT-4-class LLM responsible for decomposing high-level climate policy objectives (e.g., "Achieve net-negative emissions in India by 2060 under a USD 100/tCO₂ carbon price") into structured subtask specifications including technology scope, geographic resolution, budget envelope, and equity constraints.
- *IAM-Interface Agent*: Translates Coordinator outputs into parameterized GCAM or REMIND API calls, retrieves scenario outputs (temperature trajectories, technology adoption rates, land-use matrices), and reformats them as structured JSON for the Optimizer.
- *Quantum Optimizer Subsystem*: Receives a QUBO-encoded NET fleet allocation problem from the IAM-Interface Agent and solves it using the D-Wave Leap hybrid solver. Returns an allocation vector x^* specifying technology type, deployment scale (MtCO₂/yr), and geographic assignment for each CDR unit.
- *Critic Agent*: Evaluates the allocation vector x^* against a policy coherence rubric checking UNFCCC NDC compliance, land-use conflict indices, cost-effectiveness relative to social cost of carbon, and distributional equity metrics. Returns a structured critique with a binary approval flag and optional revision directives.

- *Synthesizer Agent*: Integrates approved allocation vectors with IAM scenario outputs to generate a human-readable policy brief, including a CDR deployment roadmap, sensitivity analysis summary, and uncertainty quantification based on 500-member Monte Carlo ensembles [11].

QUBO Formulation for NET Fleet Allocation

Let $T = \{t_1, t_2, \dots, t_{|T|}\}$ denote the set of available NET technologies, $R = \{r_1, r_2, \dots, r_{|R|}\}$ the set of deployment regions, and $Y = \{y_1, y_2, \dots, y_{|Y|}\}$ the planning timesteps (e.g., 5-year intervals from 2025–2075). The binary decision variable $x_{t,r,y} \in \{0,1\}$ indicates whether technology t is deployed in region r at timestep y . The objective is to minimize total system cost $C(x)$ subject to carbon removal target constraints, land-use bounds, and co-benefit equity conditions:

$$\text{minimize: } H(x) = H_{\text{cost}}(x) + \lambda_1 \cdot H_{\text{constraint}}(x) + \lambda_2 \cdot H_{\text{equity}}(x)$$

where H_{cost} encodes technology capital and operational expenditures, $H_{\text{constraint}}$ is a penalty term for CDR target violations encoded as squared slack variables, and H_{equity} is a penalty for Gini-coefficient deviations in regional co-benefit distribution parameterized by Lagrange multipliers λ_1 and λ_2 tuned via grid search. Reformulating continuous removal quantities through binary expansion (up to 10-bit precision per variable) yields a QUBO matrix $Q \in \mathbb{R}^{(N \times N)}$ where $N = |T| \times |R| \times |Y| \times 10$. For a representative scenario with $m=6$ technologies, $n=12$ regions, $k=11$ timesteps, $N \approx 7,920$ binary variables exceeding current hardware qubit counts and necessitating the D-Wave Leap hybrid solver's graph partitioning algorithm [12].

LLM-to-QUBO Translation Pipeline

A central technical challenge is the automated translation of free-text policy documents into QUBO coefficients. The Coordinator Agent employs a structured extraction prompt chain that: (1) parses legislation for binding numerical targets using named entity recognition; (2) resolves ambiguous commitments (e.g., "substantial CDR contribution") to calibrated quantity distributions using Retrieval-Augmented Generation (RAG) over IPCC Working Group III scenarios; and (3) maps identified constraints to penalty coefficient classes in the QUBO template. Extraction fidelity was validated against 87 manually annotated NDC documents, achieving a precision of 0.91 and recall of 0.88 on numerical target extraction [13].

EXPERIMENTAL DESIGN AND BENCHMARKING

Scenario Corpus Construction

A corpus of 1,200 policy scenarios was constructed by systematically varying five dimensions:

1. Carbon price trajectory (USD 50–300/tCO₂, 6 levels).
2. CDR target (1–10 GtCO₂/yr by 2050, 5 levels).
3. Technology availability (full portfolio, BECCS-excluded, DACCS-only, nature-based only, 4 configurations).
4. Regional scope (Global, Indo-Pacific, EU+UK, Sub-Saharan Africa, 5 regions).
5. Equity weight λ_2 (0, 0.25, 0.5, 1.0, 4 levels). Baseline IAM outputs were sourced from the IPCC AR6 Scenario Explorer (Huppmann et al., 2022) for the C1–C6 warming categories. Each scenario was independently solved by Nega Optima (quantum hybrid), a CPLEX MILP baseline, and a simulated annealing baseline [14].

Computational Environment

All experiments were conducted on a hybrid computing infrastructure comprising a D-Wave Advantage 4.1 system (5,627 qubits, Pegasus P16 topology) accessed via the D-Wave Leap cloud API, orchestrated by an on-premises server cluster (4× NVIDIA A100 80GB GPUs, 512 GB RAM, AMD EPYC 7763) for LLM inference using Llama-3-70B-Instruct quantized to 8-bit precision. GCAM version 6.0 and REMIND-MAGPIE 3.2 were deployed as containerized microservices called via HTTP API by the IAM-Interface Agent. Total end-to-end pipeline latency per scenario ranged from 8.3 to 41.7 minutes depending on complexity, compared to 45 minutes to 6.2 hours for the MILP baseline [15].

Performance Metrics

Four primary performance dimensions were assessed:

1. Solve time (wall-clock minutes to first feasible solution within 5% of optimum).
2. CDR portfolio deviation (percentage difference between Nega Optima allocation and IPCC AR6 reference pathway).
3. Land conflict index (LCI), defined as the normalized area overlap between CDR land requirements and existing food/forest/protected land designations.
4. Policy coherence score (PCS), a 0–100 composite metric evaluated by the Critic Agent incorporating UNFCCC compliance, cost-effectiveness, and distributional equity sub-scores [16].

RESULTS

Computational Performance

Table 1 summarizes mean solve-time performance across all 1,200 scenarios. Nega Optima achieved a mean solve time of 18.4 minutes, representing a 67.3% reduction relative to the CPLEX MILP baseline (56.3 minutes) and a 44.1% reduction relative to simulated annealing (33.0 minutes). Performance advantages were most pronounced for high-dimensional scenarios ($N > 5,000$ variables), where MILP solve times exceeded 4 hours while Nega Optima consistently solved within 35 minutes (Table-1).

Carbon Removal Portfolio Quality

Nega Optima's CDR portfolios exhibited a mean deviation of 4.2% from IPCC AR6 C1–C3 reference pathways, compared to 3.1% for MILP (which achieved slightly higher precision at the cost of $3\times$ longer solve times) and 8.7% for simulated annealing. Crucially, Nega Optima's portfolios demonstrated superior temporal coherence: the inter-decadal ramp rate of DACCS deployment remained within IPCC feasibility bounds in 96.8% of scenarios, versus 78.3% for simulated annealing. This is attributable to the Critic Agent's sequential approval mechanism, which explicitly penalizes deployment trajectories inconsistent with manufacturing scale-up constraints embedded in the IPCC technology readiness matrix.

Equity and Land-Use Performance

The equity-weighted QUBO formulation produced measurable improvements in distributional CDR co-benefits. Across 240 Indo-Pacific scenarios where land pressure is most acute Nega Optima's land conflict index of 0.18 represented a 14.3% improvement over MILP (0.21) and a 37.9% improvement over simulated annealing (0.29). When $\lambda_2 = 1.0$ (maximum equity weight), the Gini coefficient of co-benefit distribution across sub-national regions improved from 0.43 (unweighted) to 0.31, indicating substantially more equitable distribution of sequestration co-benefits including soil fertility, water quality, and biodiversity gains. Policy coherence scores averaged 82.4/100 under Critic Agent review, with the most frequent critique categories being: cost-optimism bias in DACCS projections (23% of flagged scenarios) and insufficient consideration of Article 6.4 mechanisms under the Paris Agreement (18%).

Table 1. Comparative computational performance across 1,200 scenario simulations.

Metric	Nega optima	CPLEX MILP	Sim. annealing	Improvement (%)
Mean solve time (min)	18.4	56.3	33.0	67.3 vs MILP
CDR portfolio deviation (%)	4.2	3.1	8.7	—
Land conflict index (LCI)	0.18	0.21	0.29	14.3 vs MILP
Policy coherence score	82.4/100	71.3/100	63.8/100	+15.6 pts
Equity gini deviation	0.043	0.071	0.119	39.4 vs MILP
Scenarios > optimality gap 5%	4.1%	12.8%	31.6%	—

DISCUSSION

Interpretability and Trust in Agentic Climate Systems

A persistent concern with AI-assisted policy systems is the opacity of decision rationales. Nega Optima addresses this through two mechanisms. First, the Coordinator Agent generates an explicit reasoning trace for each policy decomposition step, formatted as a chain-of-thought log accessible to human reviewers. Second, the Synthesizer Agent produces a structured policy brief that maps each QUBO allocation decision back to its policy justification, enabling policymakers to audit the logical chain from NDC text to deployment vector. In user evaluation studies with 14 climate policy professionals, the audit trail was rated as "sufficiently interpretable" by 78.6% of participants a meaningfully higher proportion than reported for comparable black-box IAM outputs (typically 45–55% in prior usability studies).

Quantum Hardware Limitations and Mitigation

The D-Wave Advantage architecture imposes two practical constraints relevant to Nega Optima. First, qubit connectivity is sparse: the Pegasus P16 graph has a maximum vertex degree of 15, requiring QUBO embedding that introduces ancilla qubits and chain strength penalties. For the largest problem instances ($N \approx 8,000$ variables), the embedding overhead increased the effective qubit requirement by approximately $2.3\times$, necessitating use of the hybrid solver's graph partitioning strategy. Second, thermal noise in physical qubits introduces stochastic variation: across 100 repeated annealing runs per scenario, the coefficient of variation of the objective function value was 3.8%, addressed through majority-vote aggregation of the top 10 solutions. We anticipate that gate-model quantum computing advances particularly fault-tolerant implementations of QAOA on superconducting processors will substantially reduce both limitations within the 2027–2030 timeframe.

GENERALIZABILITY AND DEPLOYMENT PATHWAY

While Nega Optima was developed and evaluated in the context of negative emission optimization, its architectural principles generalize to any domain requiring the integration of policy text parsing, combinatorial optimization, and iterative expert critique. Immediate near-term deployment pathways include national climate ministry decision-support tools, UNFCCC technical expert review augmentation, and multilateral development bank climate finance allocation systems. Barriers to deployment include data sovereignty concerns around IAM scenario data, LLM hallucination risk in low-resource language policy documents, and the absence of standardized QUBO interfaces for established IAM software. A proposed Nega Optima Deployment Readiness Framework (DRF) with seven maturity levels from prototype to operational deployment is provided in the supplementary materials.

LIMITATIONS

Nega Optima, despite its demonstrated advantages, operates under several acknowledged constraints. The QUBO binary expansion approach introduces quantization error in removal quantities; future work should explore continuous-variable quantum computing formulations via photonic or bosonic hardware. The Critic Agent's policy coherence rubric was developed for UNFCCC-aligned jurisdictions; extension to carbon markets operating under voluntary or Article 6.2 bilateral frameworks requires additional rubric development. LLM inference costs at scale (approximately USD 0.40 per complete scenario pipeline at current API pricing) may constrain deployment in low-income country policy environments a concern addressable through open-source model fine-tuning on climate policy corpora.

CONCLUSION

This paper has presented Nega Optima, the first integrated agentic AI framework combining large language model orchestration and quantum annealing for real-time negative emission technology policy simulation. Through rigorous empirical evaluation across 1,200 IPCC-aligned scenarios, Nega

Optima demonstrated a 67.3% reduction in optimization solve time, a 41% improvement in land-use equity metrics, and a policy coherence score of 82.4/100 under autonomous LLM Critic review. These results establish that the convergence of agentic AI and quantum-classical hybrid computation is not merely a theoretical aspiration but a computationally operational capability with direct relevance to the carbon budget emergency confronting global governance systems.

As the window for limiting warming to 1.5°C narrows and the scale of required CDR deployment grows, the capacity of human analysts to navigate the full combinatorial and temporal complexity of NET portfolio optimization will necessarily be augmented by advanced computational systems. Nega Optima represents a foundational step toward policy-grade AI systems capable of operating at the speed, scale, and interdisciplinary depth that the climate emergency demands. The architecture, QUBO formulations, and agent specifications described herein are released as open-source components to support further community development and independent validation.

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