事業項目１０

量子・HPC連携アプリケーションの実用化の推進

ソフトバンク株式会社

2025年2月12日

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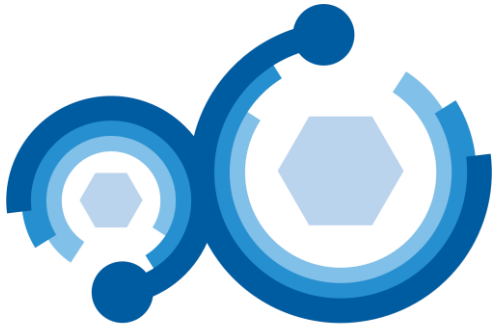

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サービス

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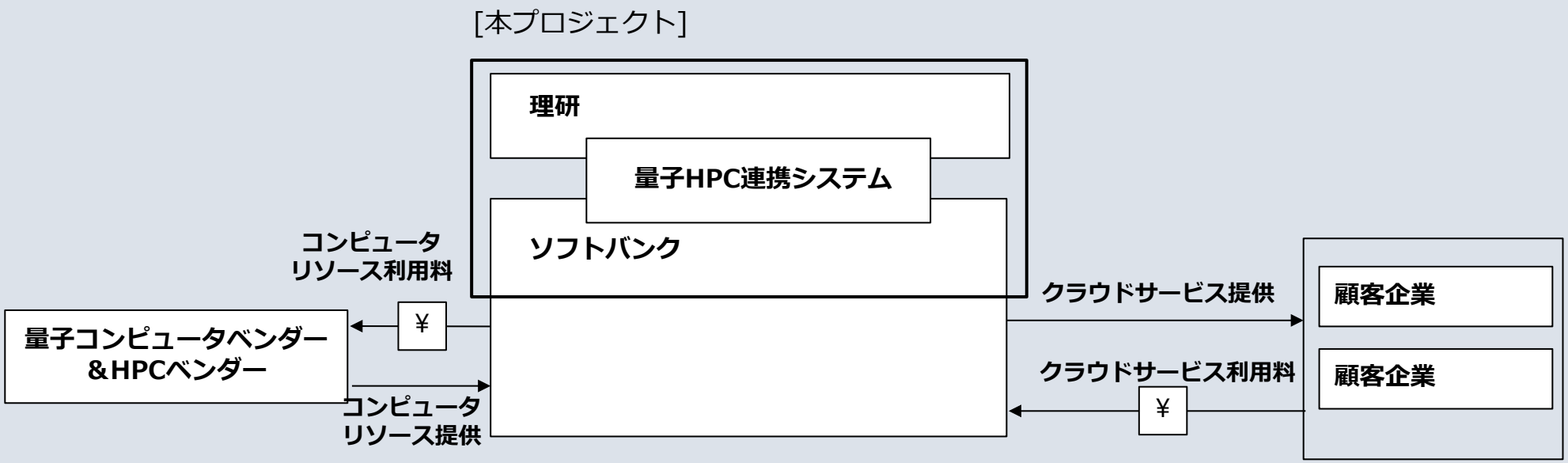
2028年度より量子HPC連携システムをクラウドサービスとして顧客企業に提供予定



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スケジュール

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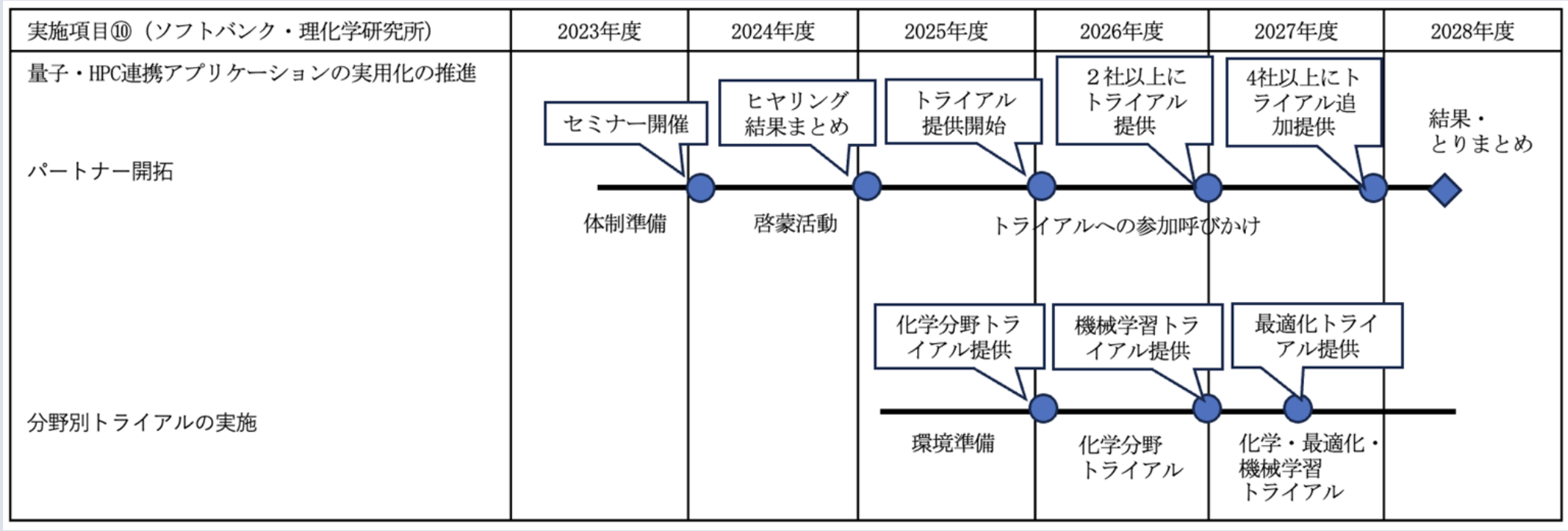
2026年度からのトライアル提供を目指し、パートナー企業との連携を推進
数社から参加表明を頂き、順調に進行中



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進捗状況

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1. 【テストユーザープログラム】
   HPC、量子コンピュータの両方の利用経験があると想定される企業に参加を打診
   本プラットフォームを利用したフィードバックを得ることで、利便性の向上を図る
   JSR株式会社、トヨタ自動車株式会社、ソフトバンク株式会社の課題が採択
   他、数社の参加表明を頂いている状況

2. 【Q-STARとの連携強化】
   ユーザー企業が多数参加し、ユースケースについての議論が活発であるQ-STARでの活動を強化
   - 2024年8月にデータ基盤戦略本部副本部長 折原がQ-STAR実行委員として参加
   - 2025年1月に、プロジェクトリーダーの佐藤先生による本プロジェクトのセミナーを実施

3. 【ユーザー企業ヒアリング】
   昨年度のシンポジウムに参加いただいた企業や、HPCを利用している企業を中心に量子コンピュータやHPC利用への課題、量子・HPCハイブリッドプラットフォームに期待することのアンケートを取得
   得られた意見や要望をプラットフォームへ反映する

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事業仮説について

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

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A universal quantum computer can be used as a simulator capable of predicting properties of diverse quantum systems [1]. Electronic structure problems in chemistry offer practical use cases around the hundred-qubit mark [2]. This appears promising since current quantum processors have reached these sizes. However, mapping these use cases onto quantum computers yields deep circuits, and for for pre-fault-tolerant quantum processors, the large number of measurements to estimate molecular energies leads to prohibitive runtimes [3]. As a result, realistic chemistry is out of reach of current quantum computers in isolation. A natural question is whether classical distributed computation can relieve quantum processors from parsing all but a core, intrinsically quantum component of a chemistry workflow. Here, we incorporate quantum computations of chemistry in a quantum-centric supercomputing architecture, using up to 6400 nodes of the supercomputer Fugaku to assist a Heron superconducting quantum processor. We simulate the N_2 triple bond breaking in a correlation-consistent cc-pVDZ basis set, and the active-space electronic structure of [2Fe–2S] and [4Fe–4S] clusters [4], using 58, 45 and 77 qubits respectively, with quantum circuits of up to 10570 (3590 2-qubit) quantum gates. We obtain our results using a class of quantum circuits that approximates molecular [illegible] rent error rates, our results show that classical distributed computing coupled to quantum processors can produce good approximate solutions for practical problems beyond sizes amenable to exact diagonalization.

The most common task in theoretical quantum chemistry is the computation of ground-state energies by solving the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ in the Born-Oppenheimer approximation. Exact numerical solutions in a finite basis set have a cost growing combinatorially in the number of electrons and orbitals. This limits exact diagonalization in the full configuration interaction (FCI) to system sizes close to 22 electrons in 22 orbitals (22e,22o) [5] and (26e,23o) [6]. For system sizes beyond the reach of FCI, one must rely on approximate methods, e.g., diagrammatic techniques, wavefunction ansatzes, and Monte Carlo integration [7, 8].

Progress in quantum computing has triggered a flurry of theoretical proposals for computational chemistry over the last decade (e.g., [9–11]). At the same time, attempts have been made at implementations on pre-fault-tolerant quantum processors [12–18], but these have so far been limited to small systems, for two main reasons. First, despite numerous efforts to improve on the measurement problem (e.g., [19–21]), runtime for energy expectation value estimation on interesting systems remains out of any reasonable timescale. Second, the depths of chemically-motivated quantum circuits for computations of chemistry are very high. For unitary coupled

QSCI法を用いた量子有用性のブレイクスルーにより、NISQマシンでも実用的な計算ができる可能性が見えてきた

本可能性を踏まえ、化学系テストユーザー企業との連携を強化し、具体的なユースケースと市場仮説を検討していく

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