Unlocking Multi-Dimensional Integration with Quantum Adaptive Importance Sampling

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Paper

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Theoretical Predictions in HEP

- Precision Era in Particle Physics: LHC and future colliders, require uncertainties in theoretical predictions that match the ever growing experimental precision.

- Theoretical predictions for high-energy colliders require going deep in QFT's perturbation theory.

- Computational Bottleneck: Prediction beyond LO requires numerical integration of multi-dimensional integrals with complicated structures.

$$\hat{\sigma}_{ab\to 1\cdots n} = \frac{1}{2\sqrt{\lambda\left((p_a+p_b)^2, m_a^2, m_b^2\right)}} \int \prod_{j=1}^{n} \frac{d^3\mathbf{p}_j}{(2\pi)^3\, 2\sqrt{\mathbf{p}_j^2 + m_j^2}} (2\pi)^4\, \delta^{(4)}\Big(p_a + p_b - \sum_{j=1}^{n} p_j\Big) \int \prod_{k=1}^{L} d^4 l_k \left| \mathscr{M}_{ab\to 1\cdots n}(\{p\},\{l\}) \right|^2$$

Phase space integrals

Multi-loop Feynman diagrams
Integrals over loop momenta

Monte Carlo and Importance Sampling

Standard Monte Carlo: By drawing N i.i.d. random samples $\{\mathbf{x}_i\}_{i=1}^{N}$, the integral is estimated by:

$$I = \int_{\Omega} f(\mathbf{x}) d\mathbf{x} \ , \qquad \hat{I}_N^{(\mathrm{MC})} = \frac{|\Omega|}{N} \sum_{i=1}^{N} f(\mathbf{x}_i) = |\Omega| \langle f \rangle \ , \ \left(\hat{\sigma}_N^{(\mathrm{MC})}\right)^2 = \frac{|\Omega|^2}{N-1} \left(\frac{1}{N} \sum_{i=1}^{N} f(\mathbf{x}_i)^2 - \langle f \rangle^2 \right) \ .$$

Importance Sampling: **Variance reduction Technique.** Using a $q(\mathbf{x})$ as the proposal Probability Density Function (PDF) that is **computationally efficient** to sample from and **resembles** $f(\mathbf{x})$.

the integral is reformulated as:

$$I = \int_{\Omega} \frac{f(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) d\mathbf{x} \ , \qquad \hat{I}_N^{(\mathrm{IS})} = \frac{1}{N} \sum_{i=1}^{N} \frac{f(\mathbf{x}_i)}{q(\mathbf{x}_i)} \ . \qquad \left(\hat{\sigma}_N^{(\mathrm{IS})}\right)^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{i=1}^{N} \frac{f(\mathbf{x}_i)^2}{q(\mathbf{x}_i)^2} - \left(\hat{I}_N^{(\mathrm{IS})}\right)^2 \right) \ .$$

VEGAS

Adaptive Importance Sampling:

- VEGAS is an Adaptive Importance Sampling Algorithm

G. P. Lepage, J. Comput. Phys. 27 (1978) 192.
G. P. Lepage, J. Comput. Phys. 439 (2021) 110386, [2009.05112].

- Generates N uniform samples in $\mathbf{y} \in [0,1]^d$ ($\mathbf{y}$ is discretised) .

- Maps to the original space: $\mathbf{y} \mapsto \mathbf{x}(\mathbf{y})$, through the Jacobian transformation: $J(\mathbf{y}) = \left| \frac{d\mathbf{x}}{d\mathbf{y}} \right|$.

$$\text{1-D grid: } \underbrace{x_0 = a,\, x_i = x_{i-1} + \Delta x_{i-1},\, x_{N_g} = b,}_{\text{Interval:}[a,b]} \quad x(y) = x_i + \Delta x_i (N_g y - i),\; i = \lfloor N_g y \rfloor,\; J(y) = N_g\, \Delta x_i\,.$$

N_g : Number of Grid cells per dimension/Constant everywhere

- The integral becomes: $I = \int_{[0,1]^d} J(\mathbf{y}) f(\mathbf{x}(\mathbf{y}))\, d\mathbf{y}$

$$\text{Integral Estimator: } \hat{I}_N^{(\text{VEGAS})} = \frac{1}{N} \sum_{i=1}^{N} J(\mathbf{y}_i) f\big(\mathbf{x}(\mathbf{y}_i)\big)$$

$$\text{Variance Estimator: } \left(\hat{\sigma}_N^{(\text{VEGAS})}\right)^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{k=1}^{N} J^2(\mathbf{y}_k) f^2\big(\mathbf{x}(\mathbf{y}_k)\big) - \left(\hat{I}_N^{(\text{VEGAS})}\right)^2 \right)$$

VEGAS

Projections:

- Entries for Jacobian for generic multidimensional transformations : $N_g^d \rightarrow$ Computationally prohibitive
- **Axis projections**: Perform the transformation on each dimension independently: $\mathbf{J}(\mathbf{y}) \rightarrow \prod_{i=1}^{d} J_i(y_i)$
- Total Degrees of Freedom: $d * N_g$
- Separable pdf: $q_{\text{VEGAS}}(\mathbf{x}) = \prod_{i=1}^{d} \sum_{k=0}^{N_g-1} \frac{1}{J_i(y_i)} \left[\Theta(x_i - x_{i,k}) - \Theta(x_i - x_{i,k+1})\right] = \prod_{i=1}^{d} q_i(x_i)$
- Efficiently finds important structures but creates **phantom structures** ,

  that lead to oversampling of irrelevant parts of the integration domain.

Quantum Monte Carlo

Typical Quantum Computational Approach:

QAE for quadratic advantage in RMSE.

A. Montanaro, Proc. R. Soc. A 471, 20150301 (2015).
C. Zoufal et al, npj Quantum Information 5 (Nov, 2019) 103.
G. Agliardi et al, Phys. Lett. B 832 (2022) 137228, [2201.01547].
K. Plekhanov et al Quantum 6 (Mar., 2022) 670.
S. Herbert ,Quantum 6 (Sept., 2022) 823
J. M. Cruz-Martinez et al, Quantum Sci. Technol. 9 (2024) 035053, [2308.05657]
J. J. M. de Lejarza, et al. Phys. Rev. D 110 (2024) 074031, [2401.03023]
J. J. M. de Lejarza et al , Quantum Sci. Technol. 10 (2025) 025026, [2409.12236]

Importance Sampling:

$$\left(\hat{\sigma}_N^{(\mathrm{IS})}\right)^2 = \frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N}\frac{f(\mathbf{x}_i)^2}{q(\mathbf{x}_i)^2} - \left(\hat{I}_N^{(\mathrm{IS})}\right)^2\right) .$$

By the number of samples, falls as: $\sigma \sim \mathcal{O}(N^{-1/2})$

Our approach:

Parenthesis Factor: Gets smaller as $q(\mathbf{x}) \to f(\mathbf{x}) \longrightarrow$ Precision critically relies on the proposal PDF

Starting Point: In HEP , that standard is the **VEGAS** algorithm

Conceptual basis:

- **Quantum Adaptive Importance Sampling (QAIS):**

Exploit the exponentially large Hilbert space of a parameterised quantum circuit (PQC) and entanglement between registers to load and sample from a non-separable proposal PDF.

- **Why Importance Sampling (IS) with Quantum Computing?**
  - IS targets small, high-impact regions.
  - Direct measurement is efficient when the answer lies in a small corner of the full Hilbert space.
  - We do not require a perfect function loading.

- **Objective:**

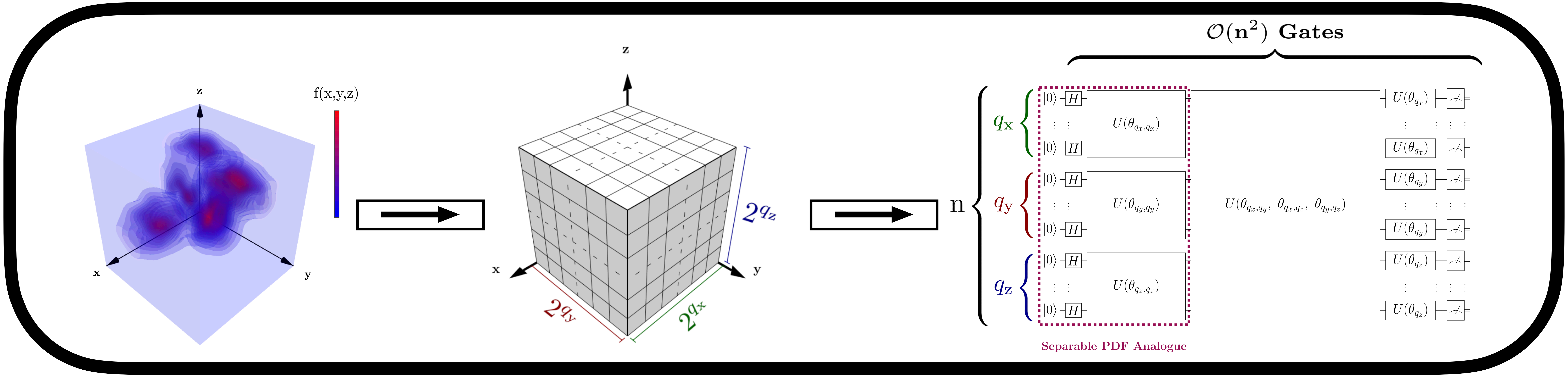
1. Reach target accuracy with fewer samples (function evaluations).

or

2. For a certain samples budget, reach better accuracy.

Quantum Adaptive Importance Sampling

Encoding:



- Domain $\Omega = \prod_{i=1}^{d} [a_i, b_i]$. Per dimension $i : q_i$ qubits $\rightarrow 2^{q_i}$ grid cells .

  Total qubits : $n = \sum_{i=1}^{d} q_i \xrightarrow{\text{Generating}} 2^n$ Grid Cells . Cell Width per dimension $i : \Omega_i = \dfrac{b_i - a_i}{2^{q_i}}$.

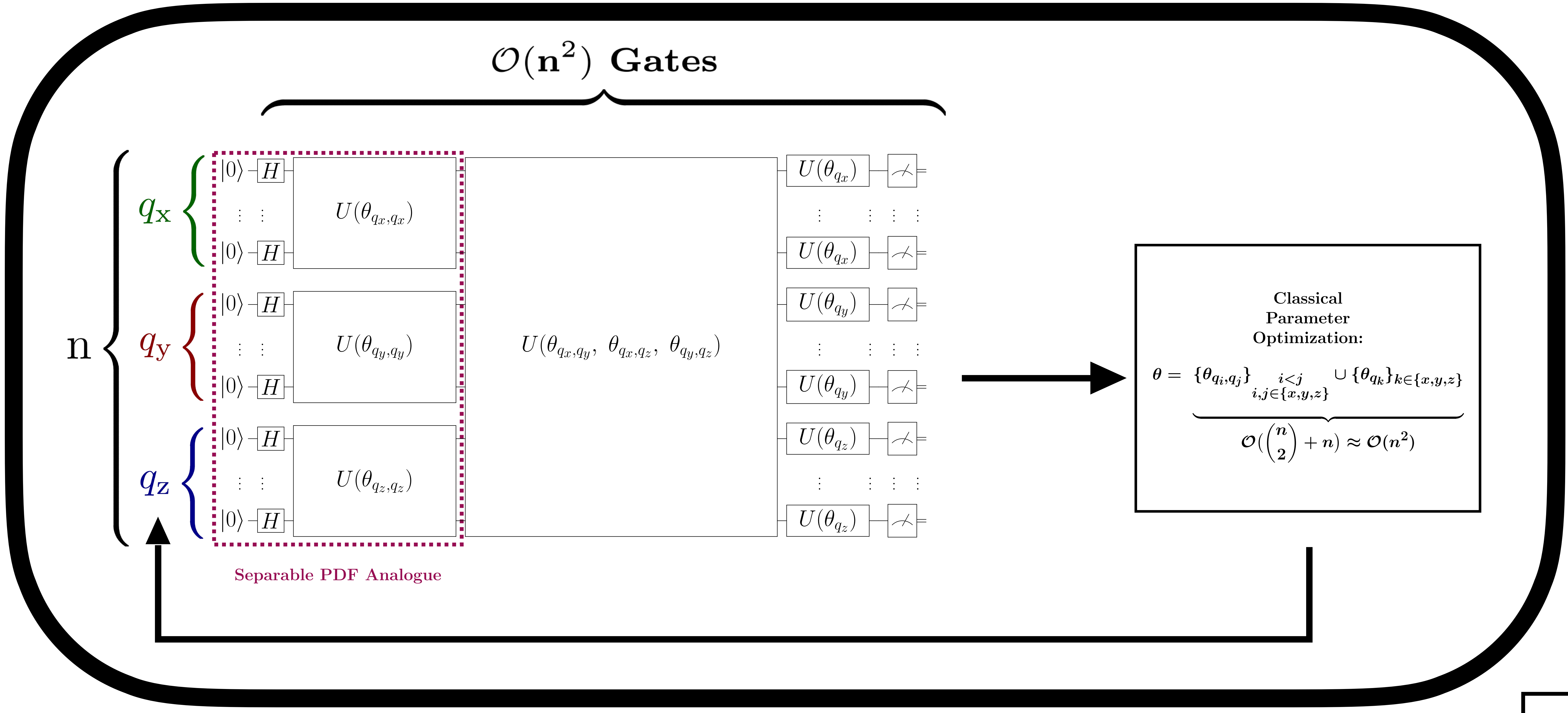
- 1-1 map between grid cells and basis states:

  State with index (Big Endian Encoding) $|j> = |j_1> \ldots |j_d> = (j_1, \ldots, j_d)$ maps to the cell: $\Omega^{(j)} = \prod_{i=1}^{d} [a_i + j_i\Omega_i, a_i + (j_i+1)\Omega_i]$

- **Proposal PDF:** $q(\mathbf{x}) = \sum_{j_1,\ldots,j_d} |c_{(j_1,\ldots,j_d)}|^2 \prod_{i=1}^{d} \frac{1}{\Omega_i}\Big[\Theta\big(x_i - (a_i + j_i\Omega_i)\big) - \Theta\big(x_i - (a_i + (j_i+1)\Omega_i)\big)\Big]$ (Generally Non-Separable)

Quantum Adaptive Importance Sampling

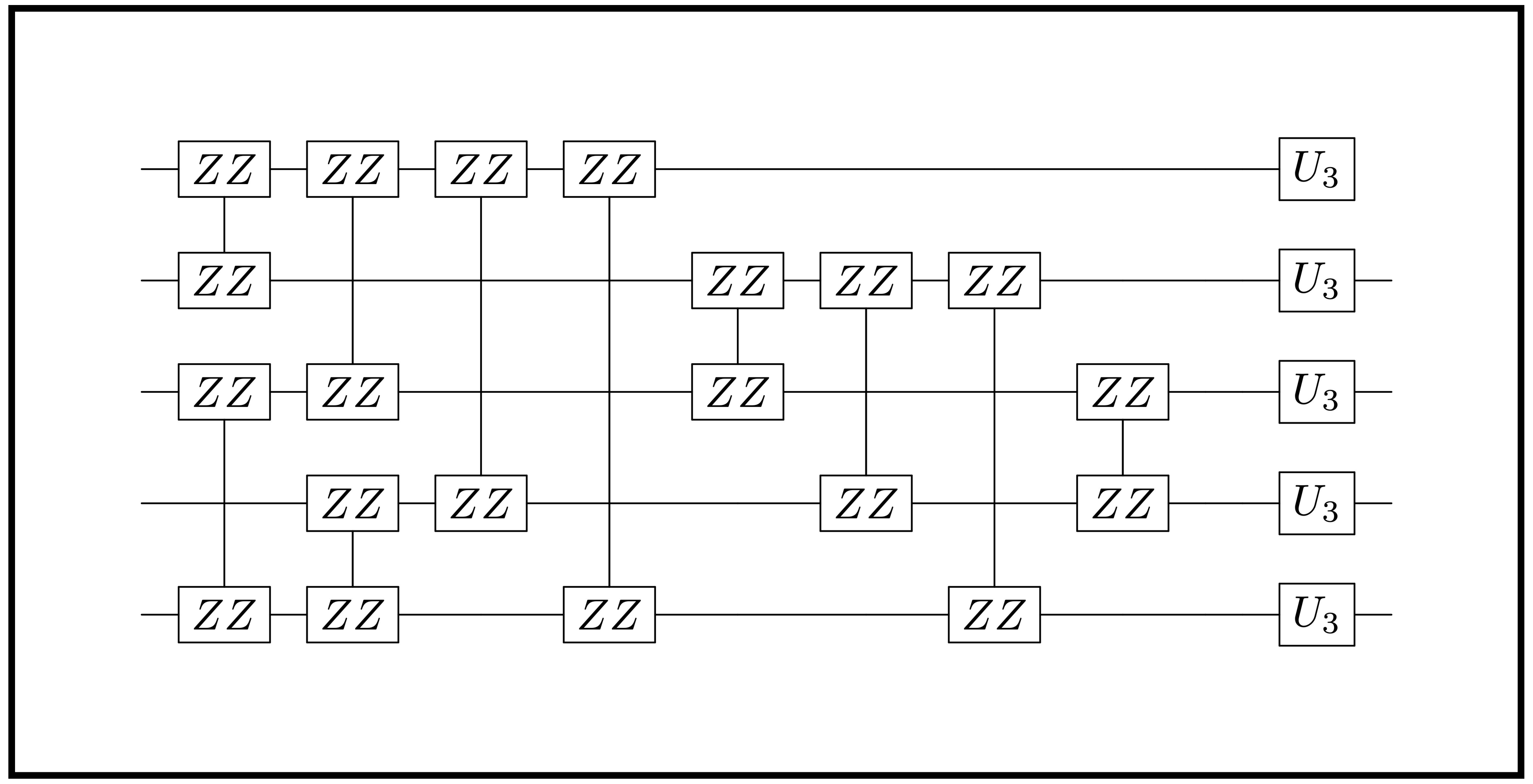
State Preparation:



- Quantum Generative Modelling for State preparation.
- SV Quantum Simulation
- Cost Function: Discretized KL-Divergence
- Optimiser: COBYLA

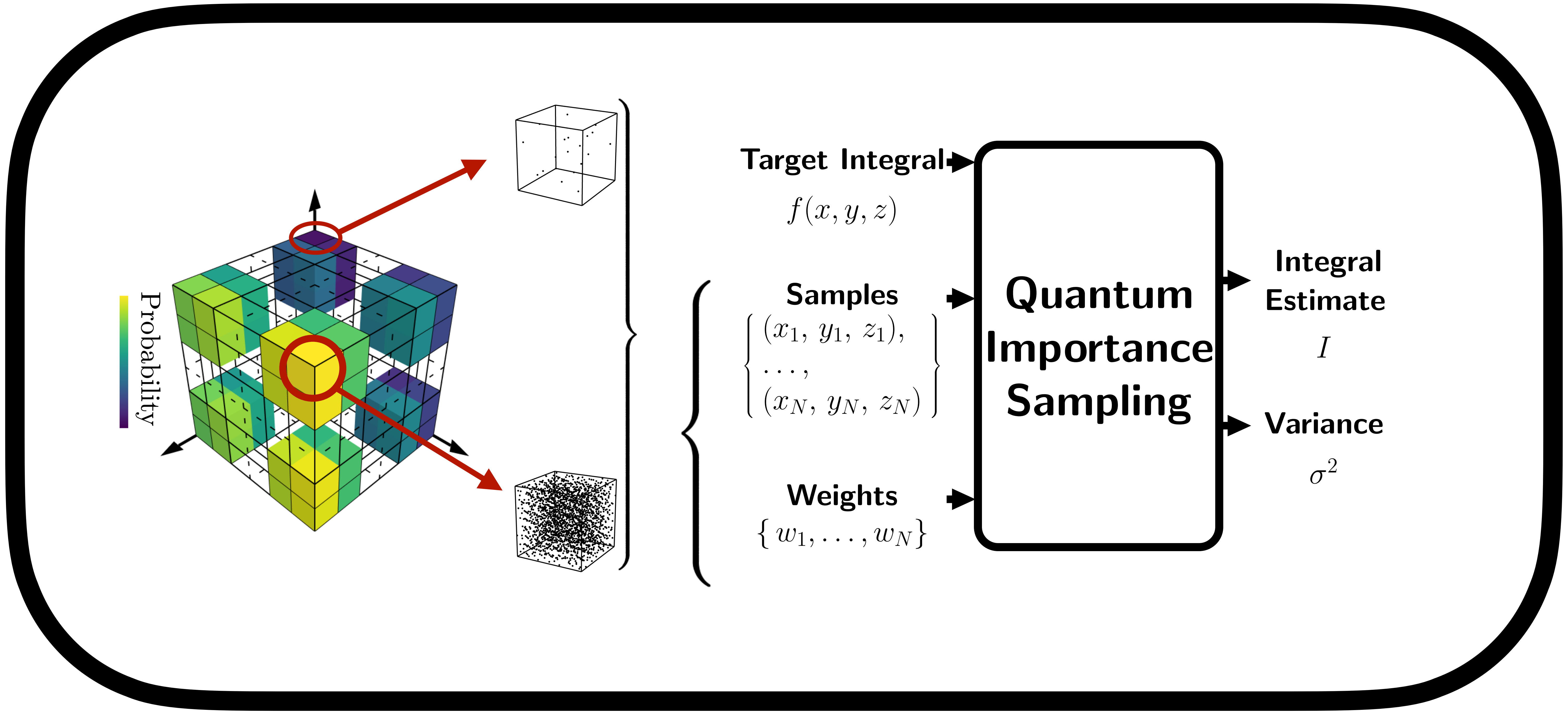
- PQC: all-to-all connectivity 2-qubit gates (QAOA-inspired):
- Number of gates and parameters: $\mathcal{O}(n^2)$:

5-Qubit Example



Quantum Adaptive Importance Sampling

Integral Estimation:



- Direct Sampling:
  N measurements.
  N_j counts per state $|j>$ or cell $\Omega^{(j)}$.
  Empirical probabilities $p_j = N_j/N$
- Empirical allocation:
  N_j points $\{\mathbf{x}_i^{(j)}\}_{i=1}^{N_j}$ drawn uniformly per cell .
- Framework fully compatible with quasi-random sequences.

- Naive Integral estimator and variance:

$$\hat{I}_N^{(\mathrm{QAIS})} = \frac{1}{N}\sum_{i=1}^{N} w^{(j)} f\left(\mathbf{x}_i^{(j)}\right), \qquad w^{(j)} = \frac{|\Omega^{(j)}|}{p_j}.$$

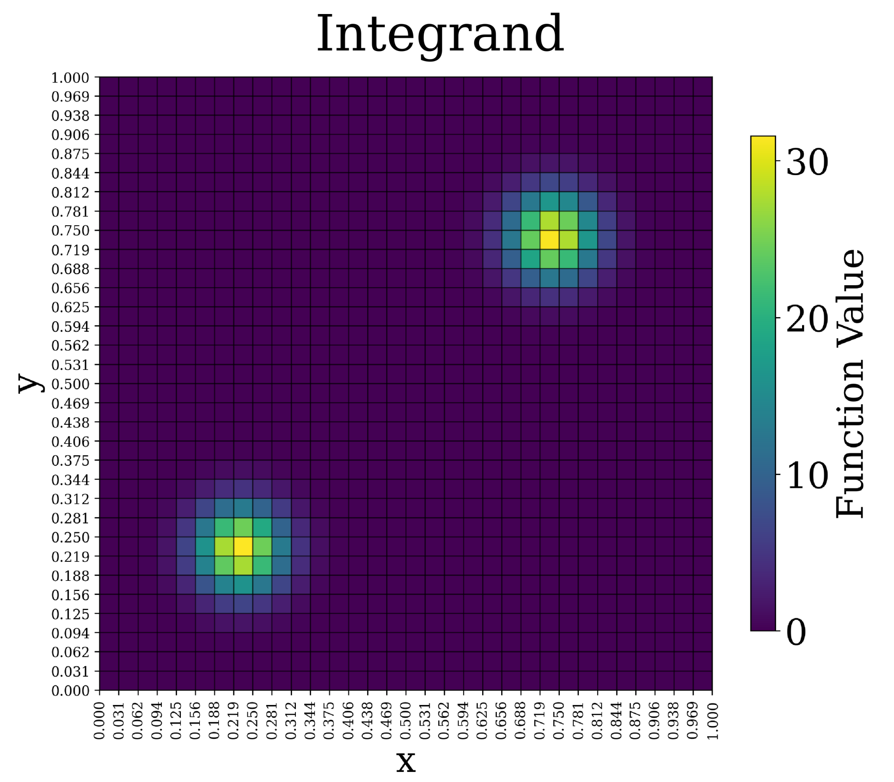
$$\left(\hat{\sigma}_N^{(\mathrm{QAIS})}\right)^2 = \frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N}\left[w^{(j)} f(\mathbf{x}_i^{(j)})\right]^2 - \left(\hat{I}_N^{(\mathrm{QAIS})}\right)^2\right)$$

$\Omega^{(j)}$: j-th grid cell $\equiv$ j-th quantum state
$\mathbf{x}_i^{(j)}$: i-th random point at grid cell j
N: Number of shots
N_j: Number of times state j was measured

Quantum Adaptive Importance Sampling

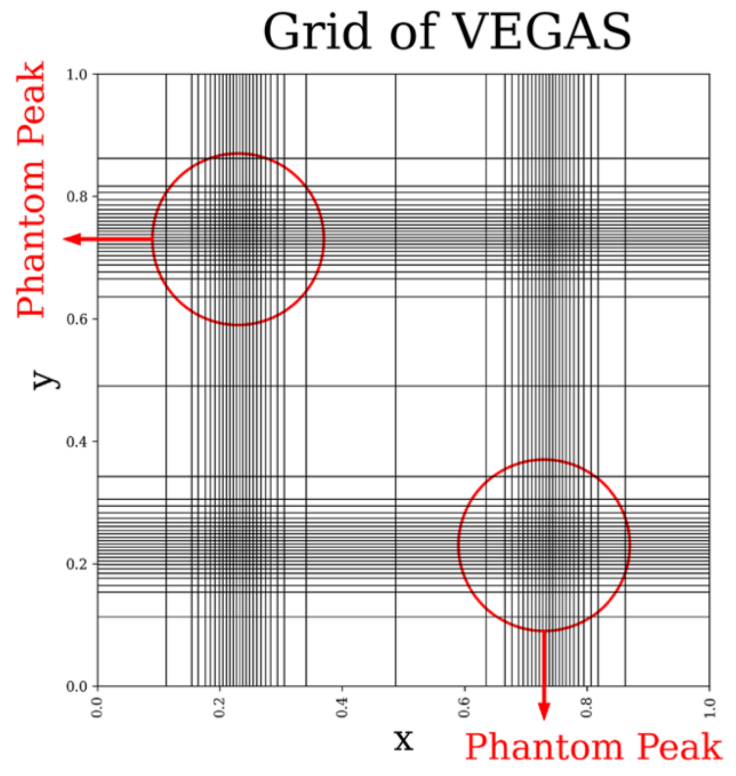
Two-Dimensional Gaussian Case:

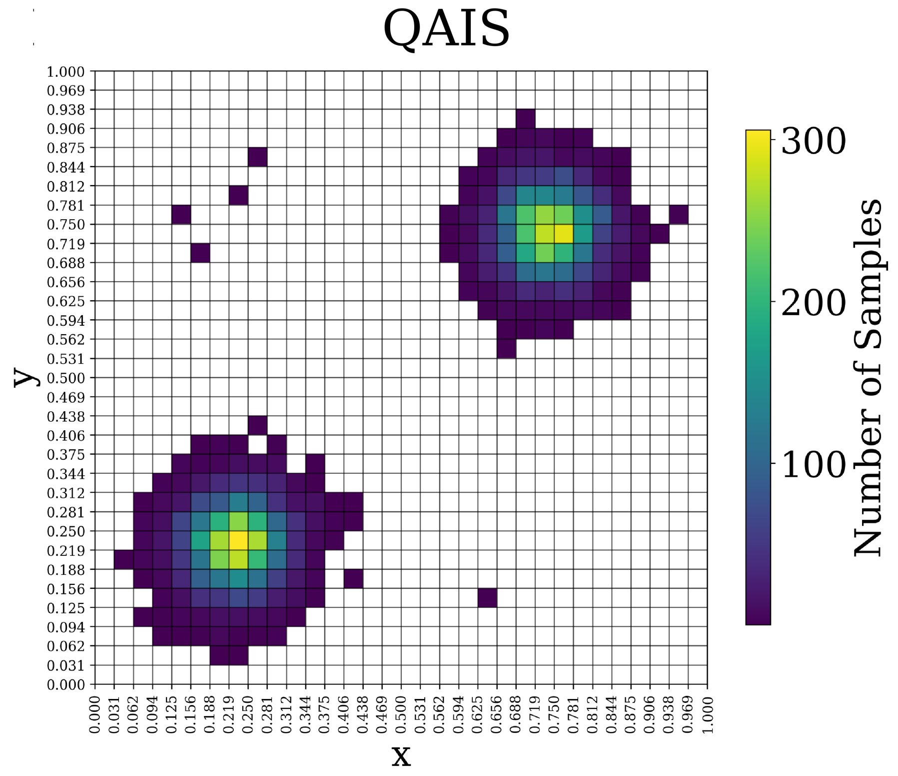
$$\int_{[0,0]}^{[1,1]} f(\mathbf{x})d\mathbf{x} = \int_{[0,0]}^{[1,1]} \left(\sum_{i=0}^{1} e^{\left(-200|\mathbf{x}-\mathbf{r}_i|^2\right)} \right) d\mathbf{x} \ , \qquad \mathbf{r}_0 = (0.23,0.23), \quad \mathbf{r}_1 = (0.74,0.74)$$

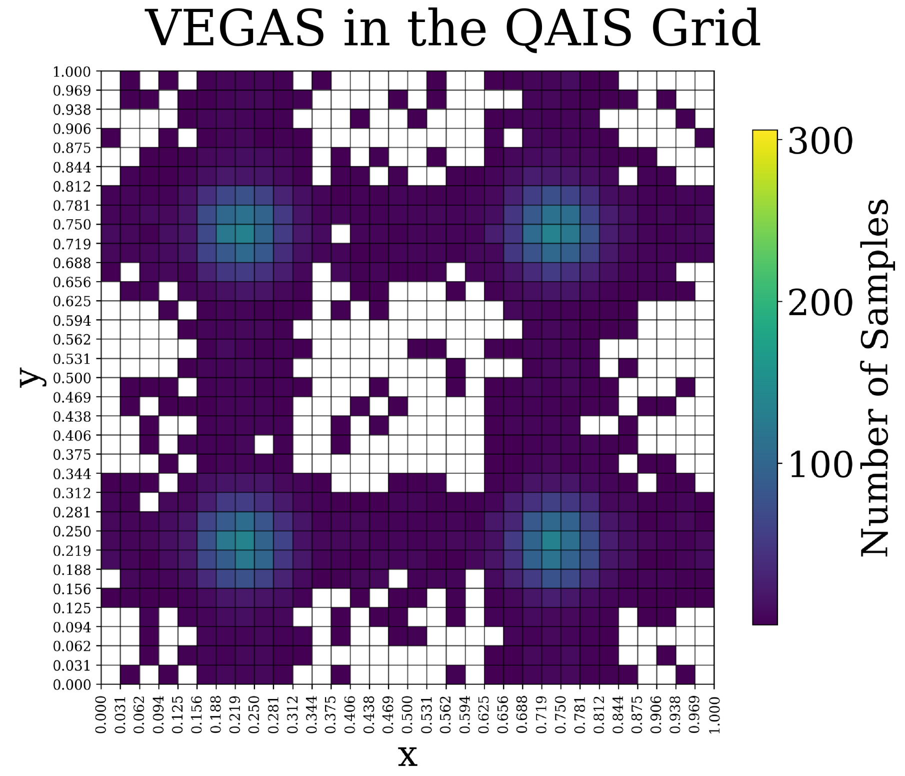


Number of Qubits: $n = 10$

Number of Shots: $N = 10^4$







- Given M **observed states out of** 2^n:

  These correspond to a region $\Omega^- \subset \Omega$

  Using the j-th cell estimator: $\hat{I}_j = \dfrac{|\Omega^{(j)}|}{N_j} \displaystyle\sum_{i=1}^{N_j} f\left(\mathbf{x}_i^{(j)}\right)$

- We observe a **systematic bias**:

$$\text{Bias} = -\sum_{j \in \Omega \setminus \Omega^-} I_j$$

Quantum Adaptive Importance Sampling

Systematic Bias Solution: Tiling Algorithm

1. Challenge: Unmeasured states → Integral underestimation (Bias)

2. Conflicting objectives:

- **Efficient Quantum Measurement:** Target at few states
- **Unbiasedness:** Evaluate every grid cell

3. Solution: **Tiling Algorithm** to reconstruct PDF over the full integration domain: $\mathcal{O}\Big(\underbrace{n\,M\,\log M}_{\text{Sorting}} + \overbrace{M\,d^3\,n^2}^{\text{Greedy Expansions}}\Big)$

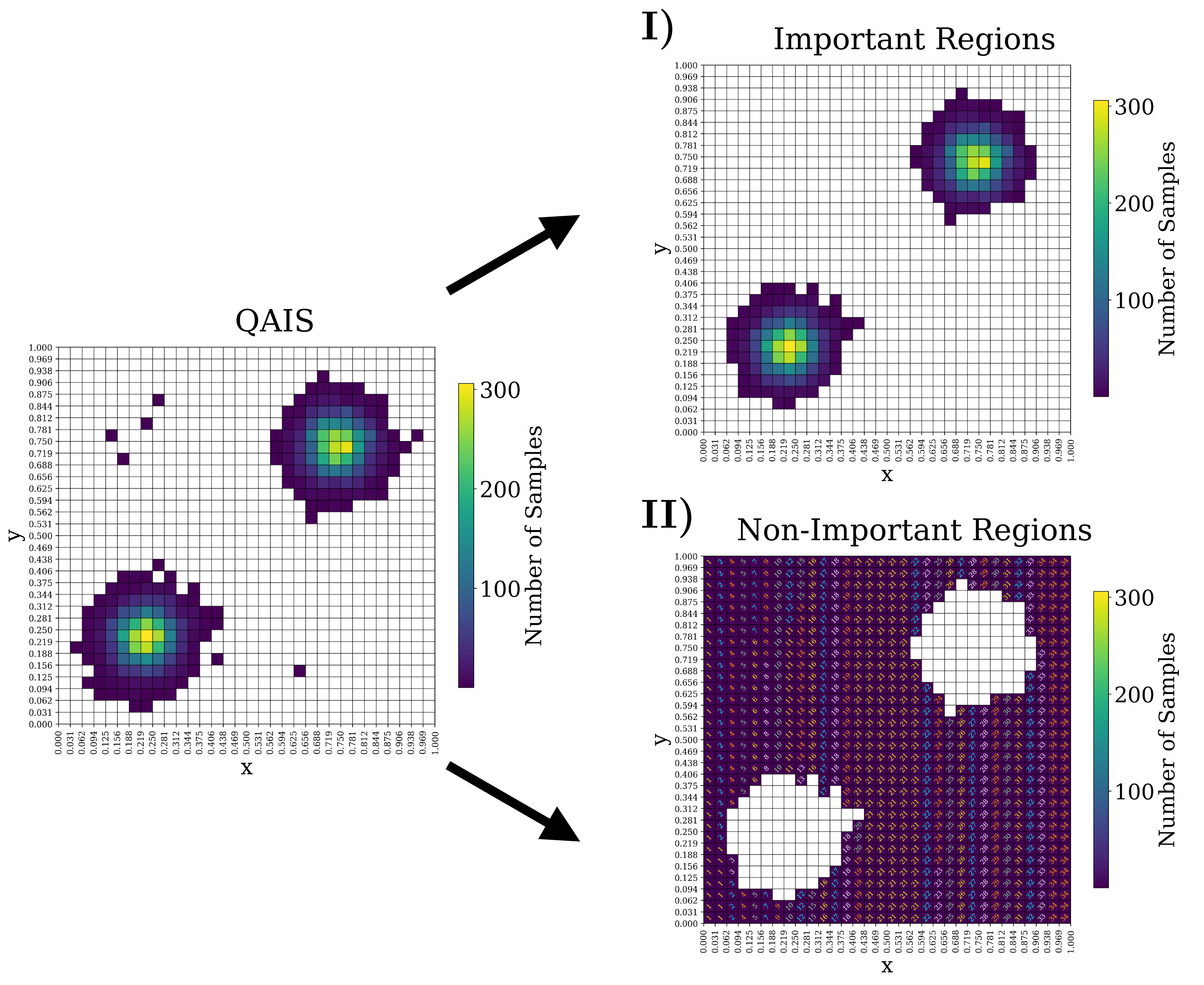
I) Detailed sampling in Important Regions

II) Sparse uniform sampling in the Non-Important Region

Contains Formerly Missing Contribution

QAIS estimator: $$\hat{I}_N^{(\mathrm{QAIS})} = \frac{1}{N}\sum_{i\in\Omega_I} w^{(i)} \sum_{j=1}^{N_i} f(\mathbf{x}_j^{(i)}) + \boxed{\frac{1}{N}\sum_{k\in\Omega_{N-I}} \tilde{w}^{(k)} \sum_{j=1}^{\tilde{N}_k} f(\mathbf{x}_j^{(k)})}$$

Practical Demonstration



Quantum Adaptive Importance Sampling

More Two-Dimensional Examples:

- Sampling efficiency of QAIS compared to VEGAS depends heavily on the target integrand's structure.

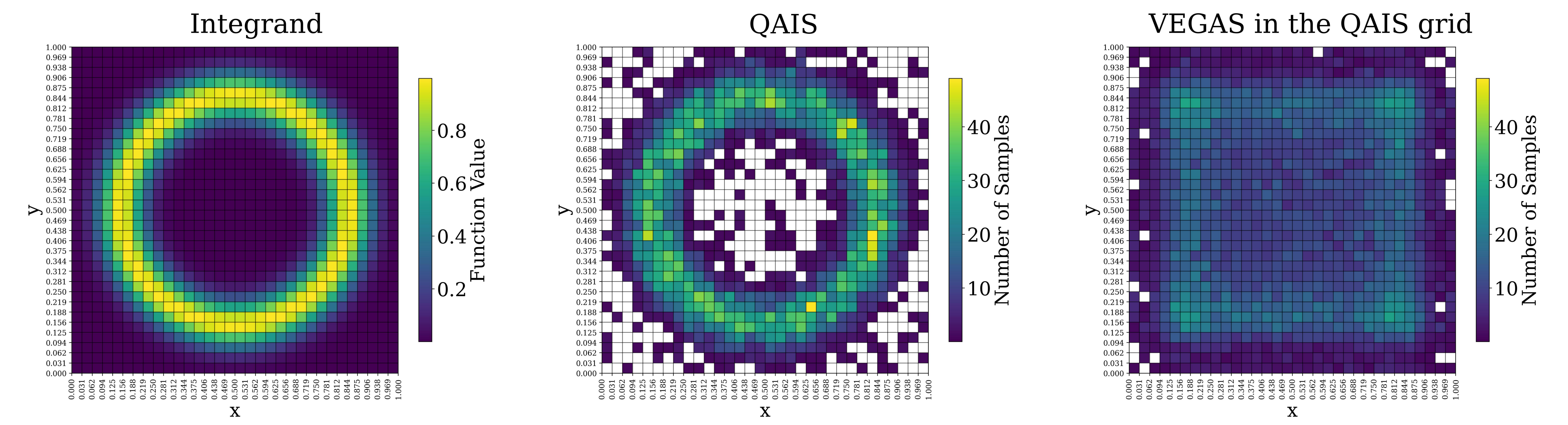
Number of Qubits: $n = 10$

Number of Shots: $N = 10^4$

Ring-Shaped Structure:

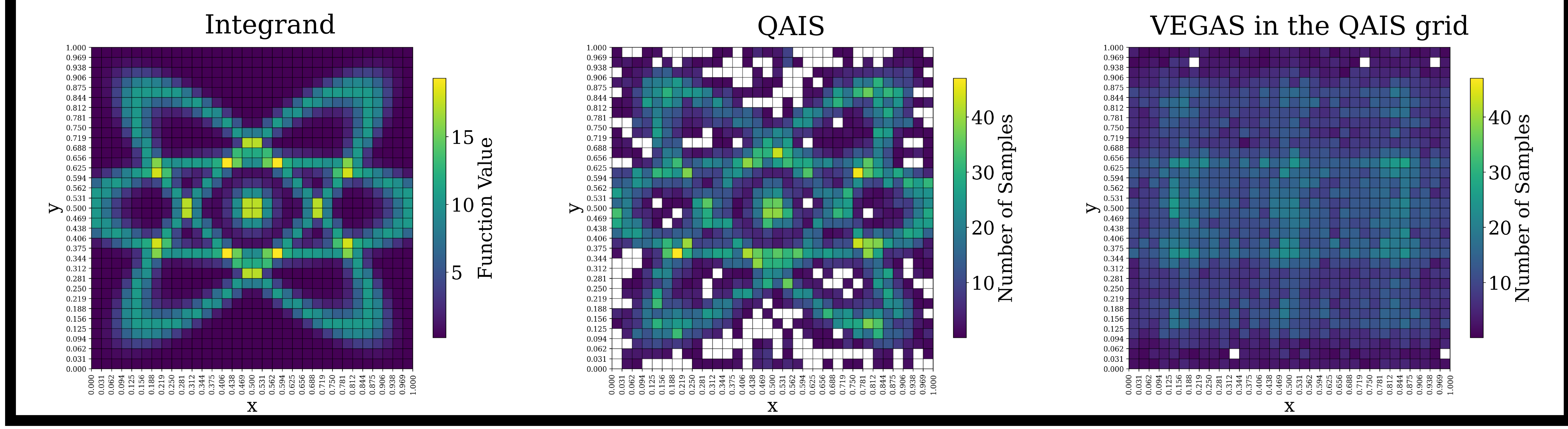
$$f_R(x, y) = e^{-k\left(\sqrt{(x-c_x)^2+(y-c_y)^2}-\rho\right)^2}$$

With: $c_x = \frac{1}{2}$, $c_y = \frac{1}{2}$, $\rho = 0.35$, $k = 200$



Atom-Shaped Structure:

$$f_A(x, y) = c_g\, e^{-(u(x)^2+v(y)^2)/(2\, s_g^2)} + \sum_{\theta\in\{0,\pi/4,-\pi/4\}} \left[c_0 + c_\theta\, e^{-(r_e(x,y,\theta)-1)^2/(2\, s_r^2)}\right]$$



With: $u(x) = x - \frac{1}{2}$, $v(y) = y - \frac{1}{2}$,

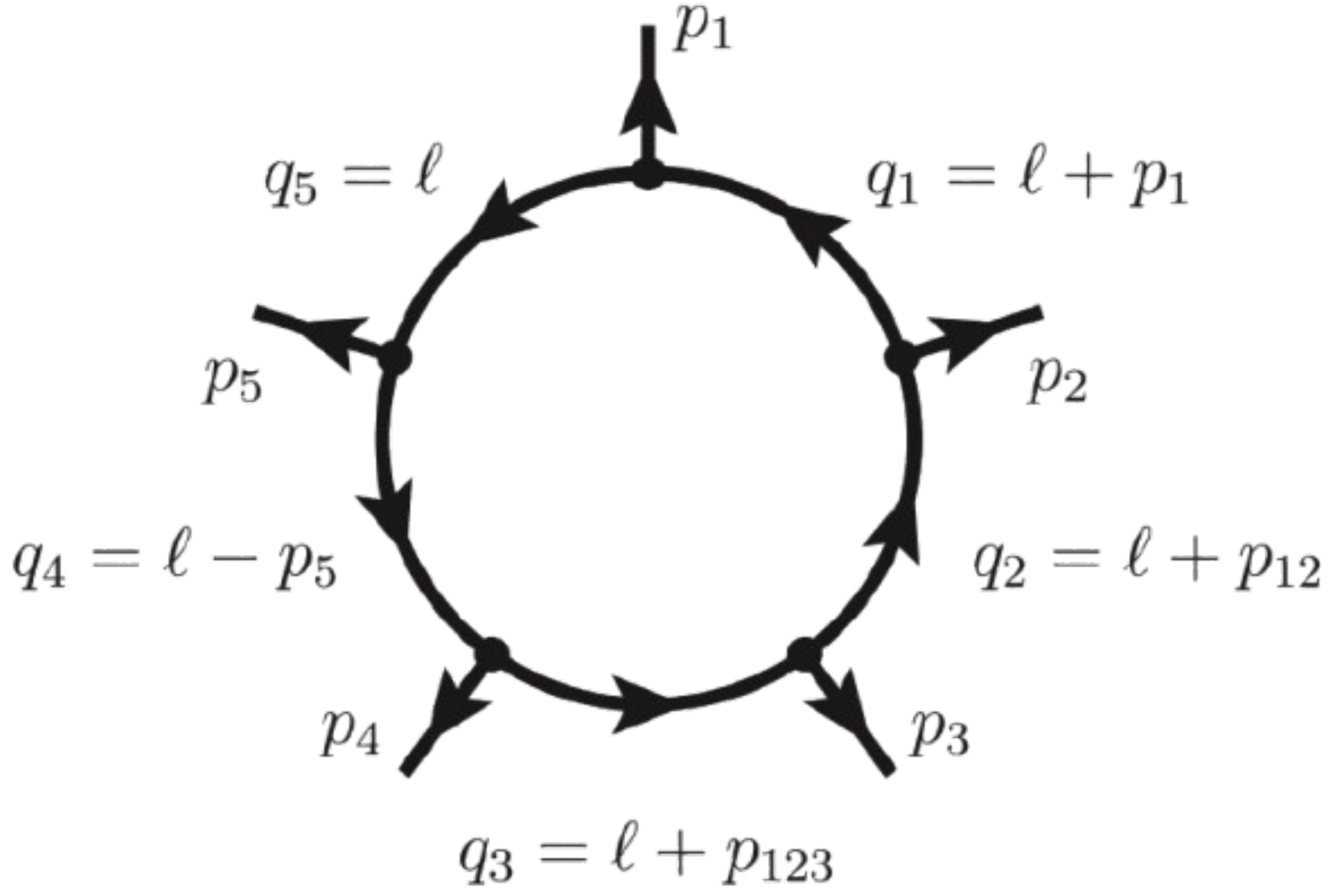
$$r_e(x, y, \theta) = \sqrt{\left(U(x, y, \theta)/a\right)^2 + \left(V(x, y, \theta)/b\right)^2}$$

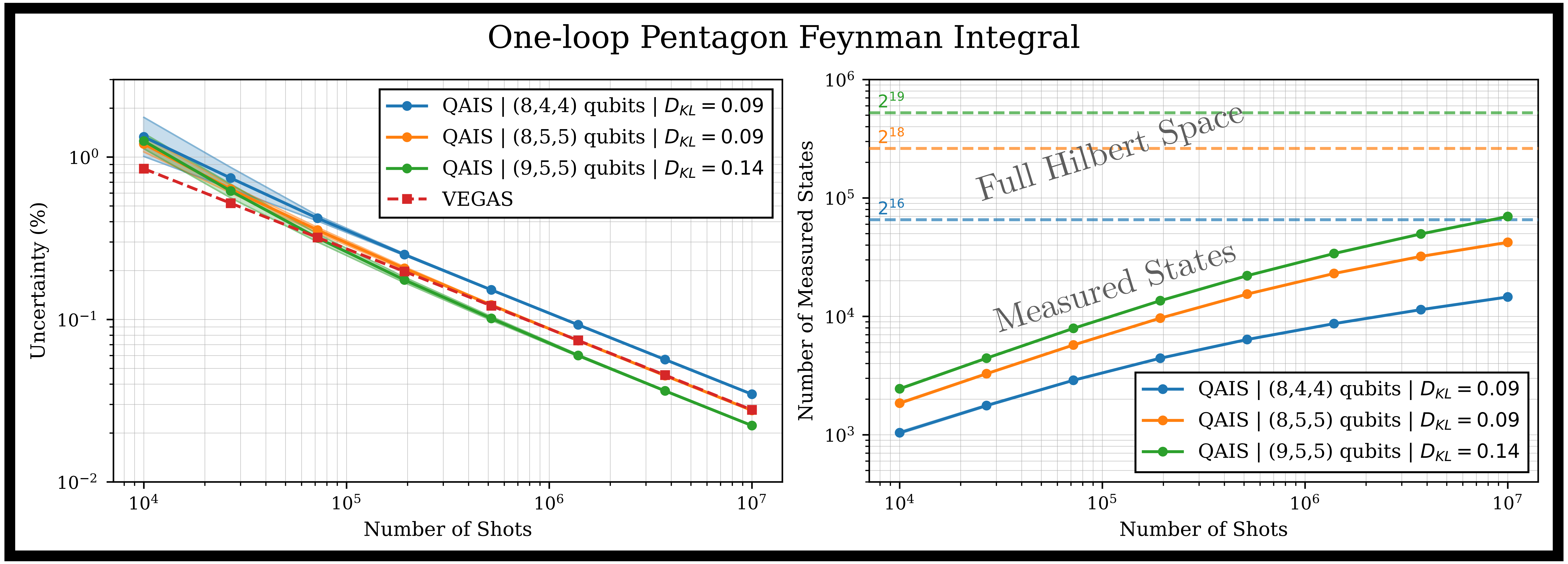
$$U(x, y, \theta) = \cos\theta\, u(x) + \sin\theta\, v(y), \qquad V(x, y, \theta) = -\sin\theta\, u(x) + \cos\theta\, v(y),$$

$a = \frac{1}{2}$, $b = 0.15$, $s_r = 0.1$, $s_g = 0.04$, $c_g = 20$, $c_0 = 0.05$, $c_\theta = 10.5$

HEP example: One-loop Pentagon

One-Loop Pentagon Diagram :
(Loop-Tree Duality)





- Uncertainty: σ/I
- Dicretization: 16-19 qubits
- Comparison made on best VEGAS proposal against best QAIS proposal
- Error bands coming form 100 independent integrations, with the same proposal PDF

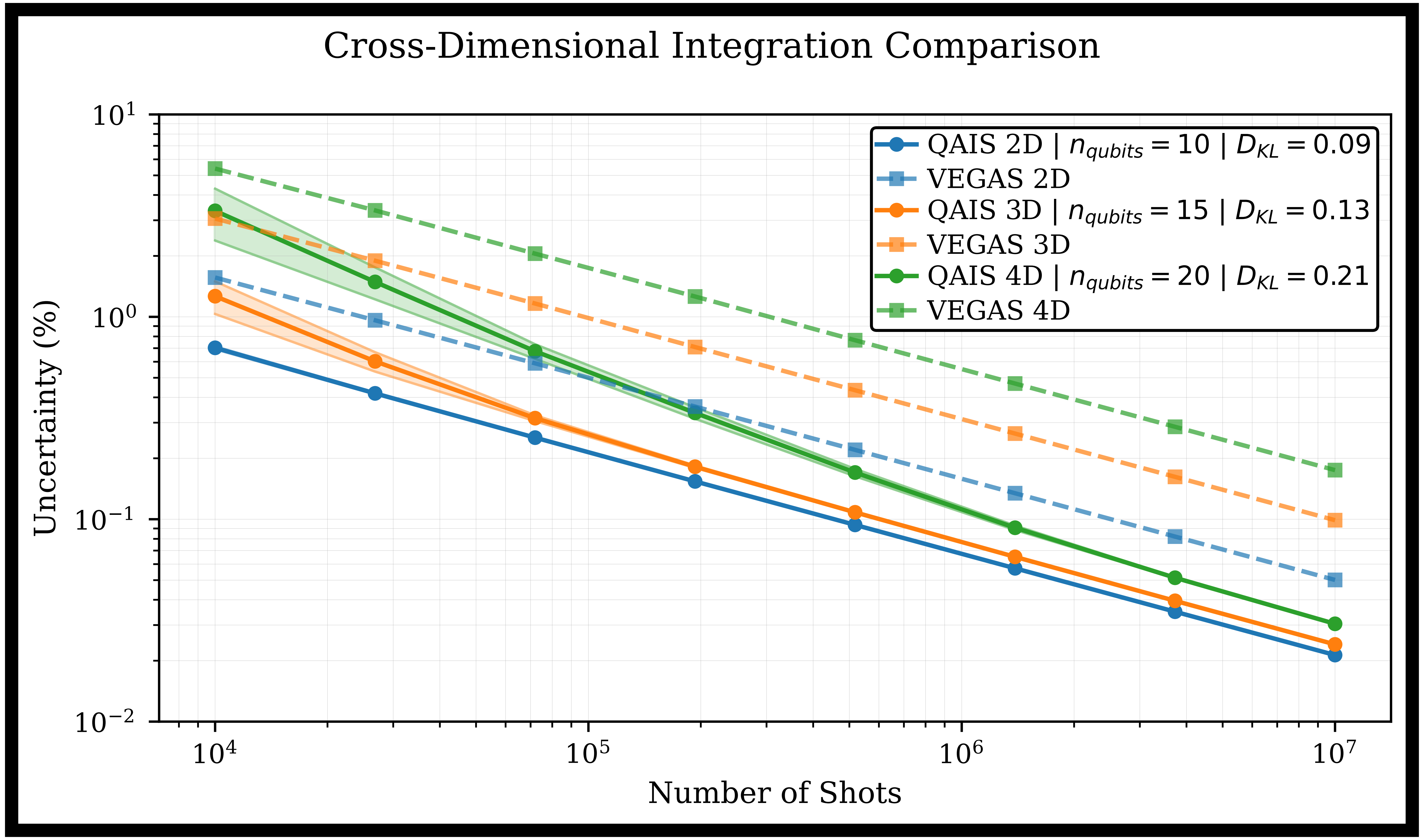
Quantum Adaptive Importance Sampling

Cross-Dimensional Results:

- Integrate the same multi-peak structure in different dimension.
- Analytic Expression:

$$\int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} = \int_{[0,1]^d} \left(\sum_{i=0}^{2} e^{-50|\mathbf{x}-\mathbf{r}_i|} \right) d\mathbf{x}$$

$\mathbf{r_0} = (0.23,\ldots,0.23), \quad \mathbf{r_1} = (0.39,\ldots,0.39), \quad \mathbf{r_2} = (0.74,\ldots,0.74)$



Integrand Dimension: 2-4 dimensions

Discretisation: 5 qubits/dimension

Approx. : 100 COBYLA iters / parameter

- We expect the precision to be governed by how well the proposal fits the target
- The main driving force should be the KL divergence
- We see that as the dimension rises , VEGAS' best grid falls behind , while QAIS is able to keep uncertainty low, particularly in the region above

Summary

- **VEGAS:** Uses a separable proposal $q_{\text{VEGAS}} = \prod_{i=1}^{d} q_i$. Reduces the grid handling DoF $N_g^d \rightarrow dN_g$.

Captures the important regions, but generates phantom structures, reducing performance.

- **QAIS:** Uses the exponential Hilbert space of a PQC and entanglement to handle the PDF over the grid and captures cross-dimensional correlations.

- **Debiasing:** Tiling removes systematic bias caused by unseen cells.

- **Results:**

  In a comparison between best proposals:

  1. Single peak function: Competitive with VEGAS.
  2. Multi-modal structure: QAIS is able to maintain small uncertainties regardless of integral's dimensionality

- **Limitations and Future work**: Limitations on arbitrary quantum state preparation. Particularly considering ongoing limitations in Quantum Machine Learning. Plan to formalise the optimisation process.

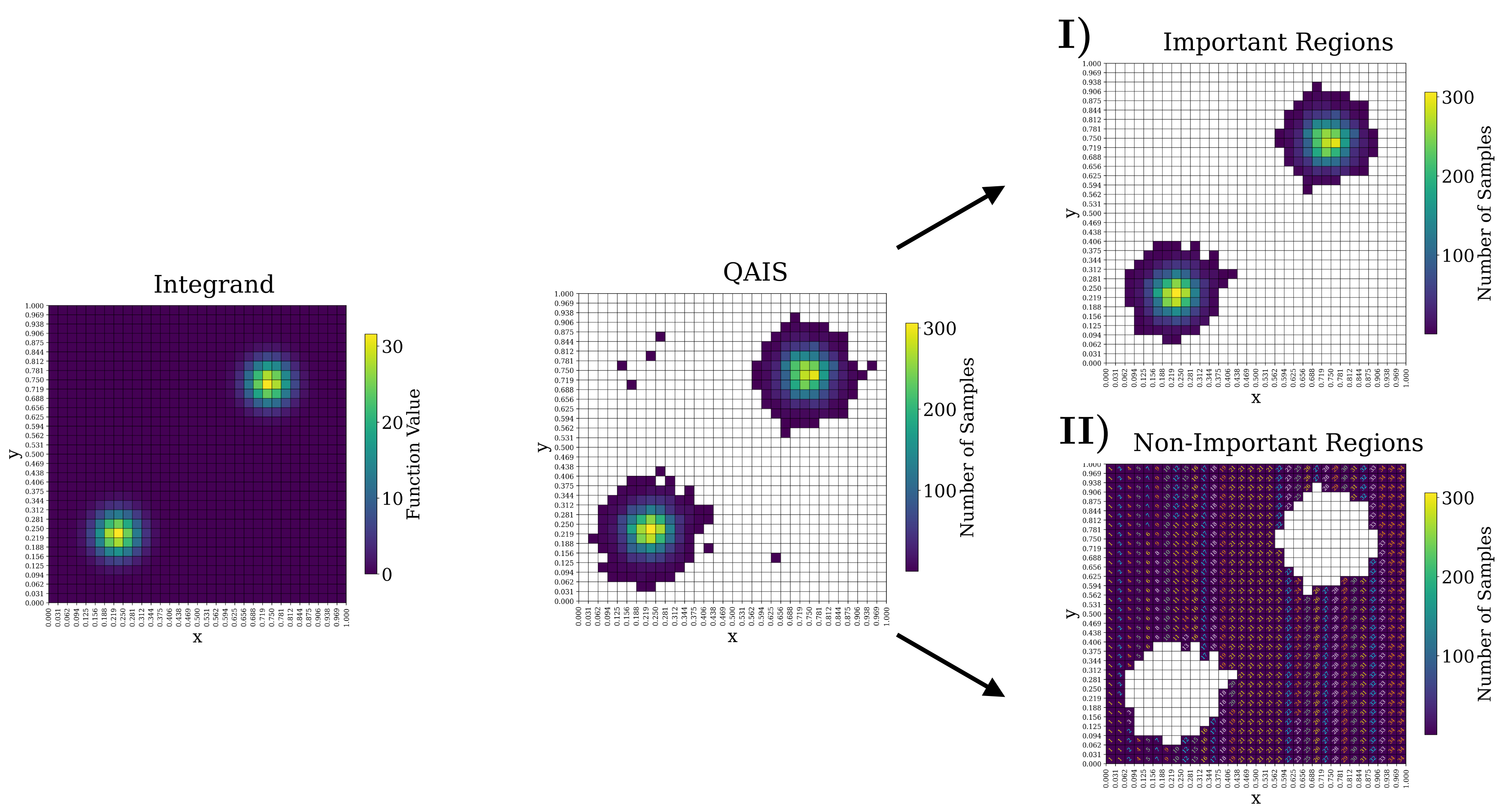
Supplementary Material

Quantum Adaptive Importance Sampling

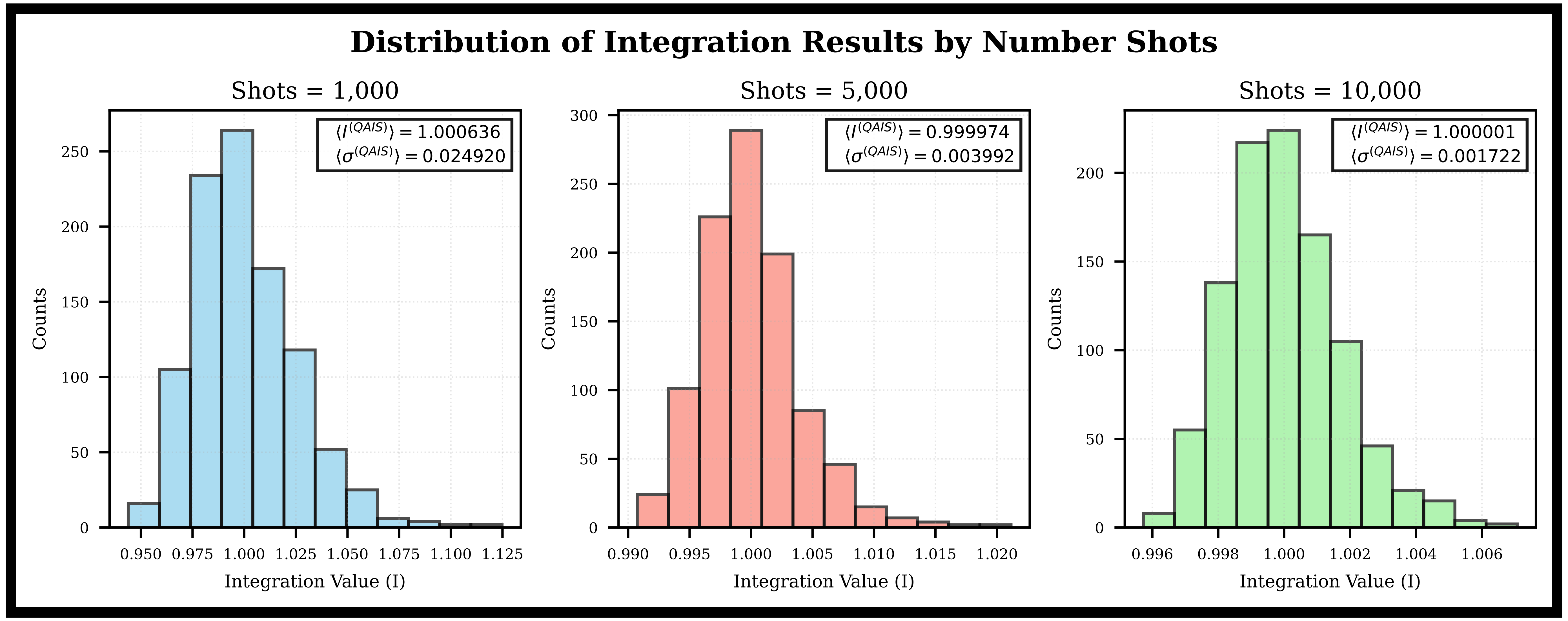
Two-Dimensional Gaussian Case: Bias check

$$\int_{[0,0]}^{[1,1]} f(\mathbf{x})\, d\mathbf{x} = \int_{[0,0]}^{[1,1]} \left(\sum_{i=0}^{1} e^{\left(-200|\mathbf{x}-\mathbf{r}_i|^2\right)} \right) d\mathbf{x}\,, \qquad \mathbf{r}_0 = (0.23,0.23), \quad \mathbf{r}_1 = (0.74,0.74)$$

Number of Qubits: $n = 10$



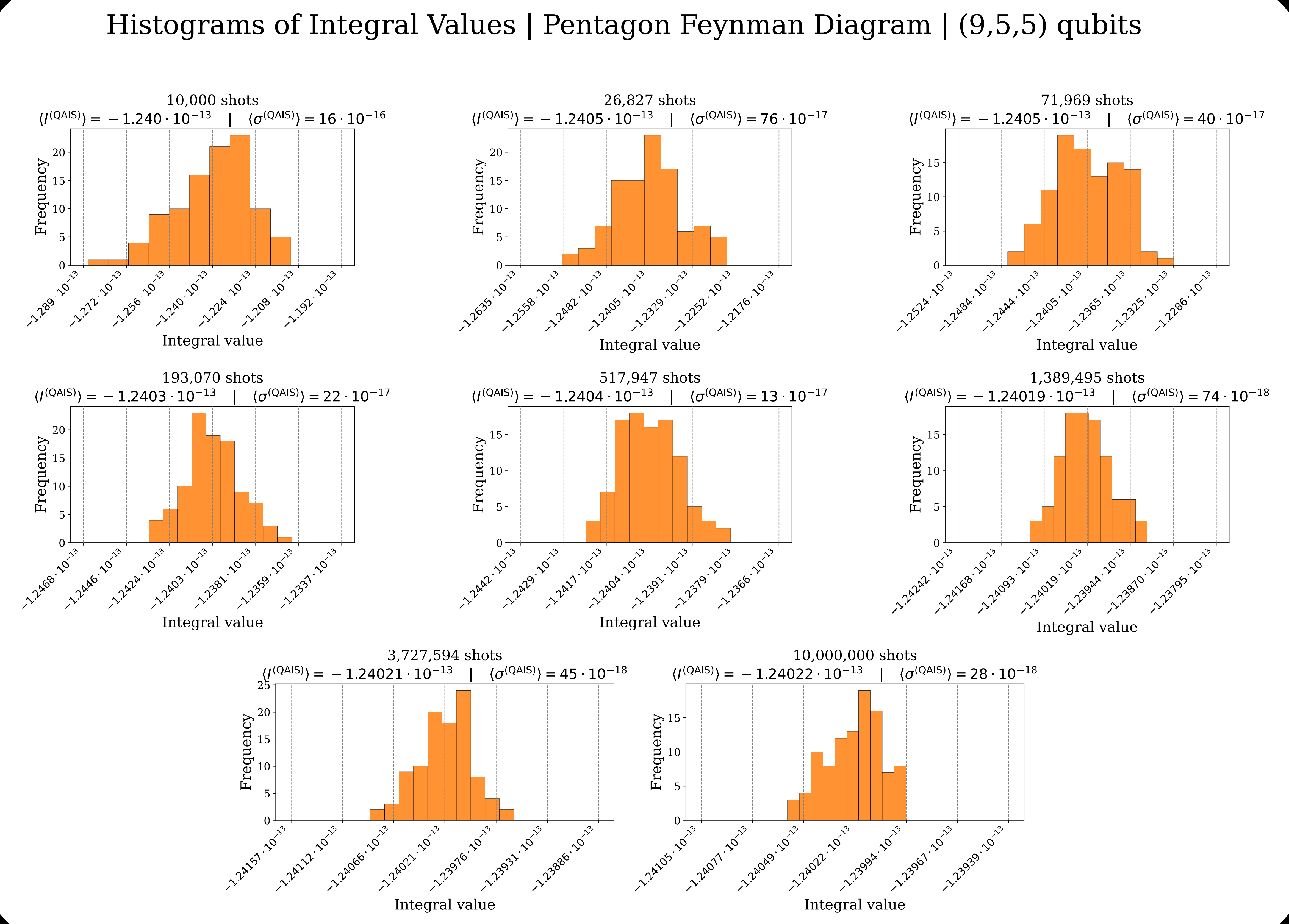
1000 Integrations with the same proposal



Quantum Adaptive Importance Sampling

Impact of Quasi-Random Sequences

Pseudo-Random (Marsenne Twister)



Quasi-Random (Sobol Sequence)