Quantum Software Engineering (QSE) in intelligent robotic cognitive control

Quantum Computational Intelligence Supremacy and Quantum Control

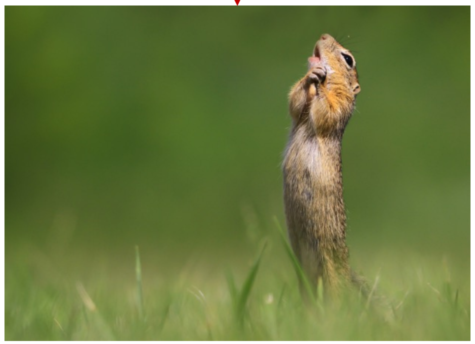
Perspective of collaboration development between JINR and IN2P3 in the next decades

1. Definition and structure of QSE

2. Quantum computational intelligence toolkit

3. Quantum Software Engineering in JINR projects

Measurement result of quantum computing



Superposition

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18 May 2021

Prof. Sergey V. Ulyanov：*略歴*

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"Statistical analysis of seismic excitation on dynamical systems with random time-dependent parameters"
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経歴

1965　Moscow State Technical University (Bauman Technical College)
1971　（自動制御システム）　入学　同上　卒業 (кафедра П -1: Системы управления)
1965 ~ 75　**Research Engineer and Senior Manager**
Central Institute of Building Construction, Ministry of Building Construction
1975 ~ 83　**Chief of Laboratory**
Central Institute of Biomedical Engineering, Ministry of Biomedical Engineering
1983 ~ 92　**Professor, Chief** of Department of Quantum and Relativistic Control Systems
Institute of Physical -Technical Problems, Soviet Academy of Sciences
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Institute for Problems in Mechanics, Russian Academy of Science

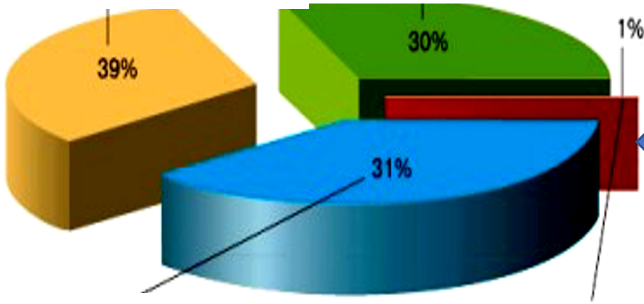
1994 ~ 97　教授
電気通信大学　機械制御工学科
1997 ~ 2007 ヤマハ発動機（株）　研究開発センター
1999 ~ 2018 同社　YMENV R&D Office in Crema (Italy)

1. Definition and structure of QSE

Jianjun Zhao (2020), Quantum Software Engineering Landscapes and Horizons https://arxiv.org/pdf/2007.07047.pdf)

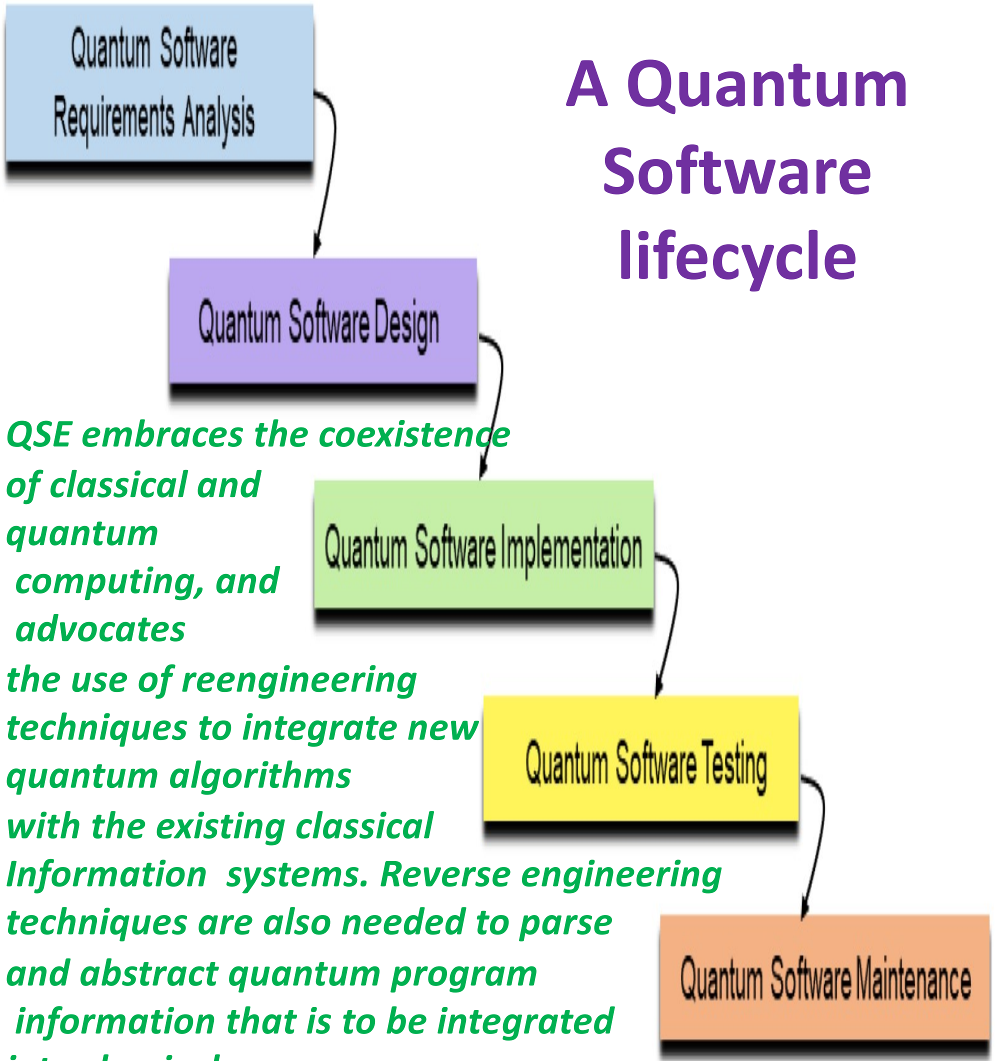
Software Engineering (SE) (Friedrich L. Bauer):
The establishment and use of sound engineering principles in order to obtain economically software that is reliable and works efficiently on real machines

Quantum software engineering (QSE) is the use of sound engineering principles for the development, operation, and maintenance of quantum software and the associated document to obtain economically quantum software that is reliable and works efficiently on quantum computers.



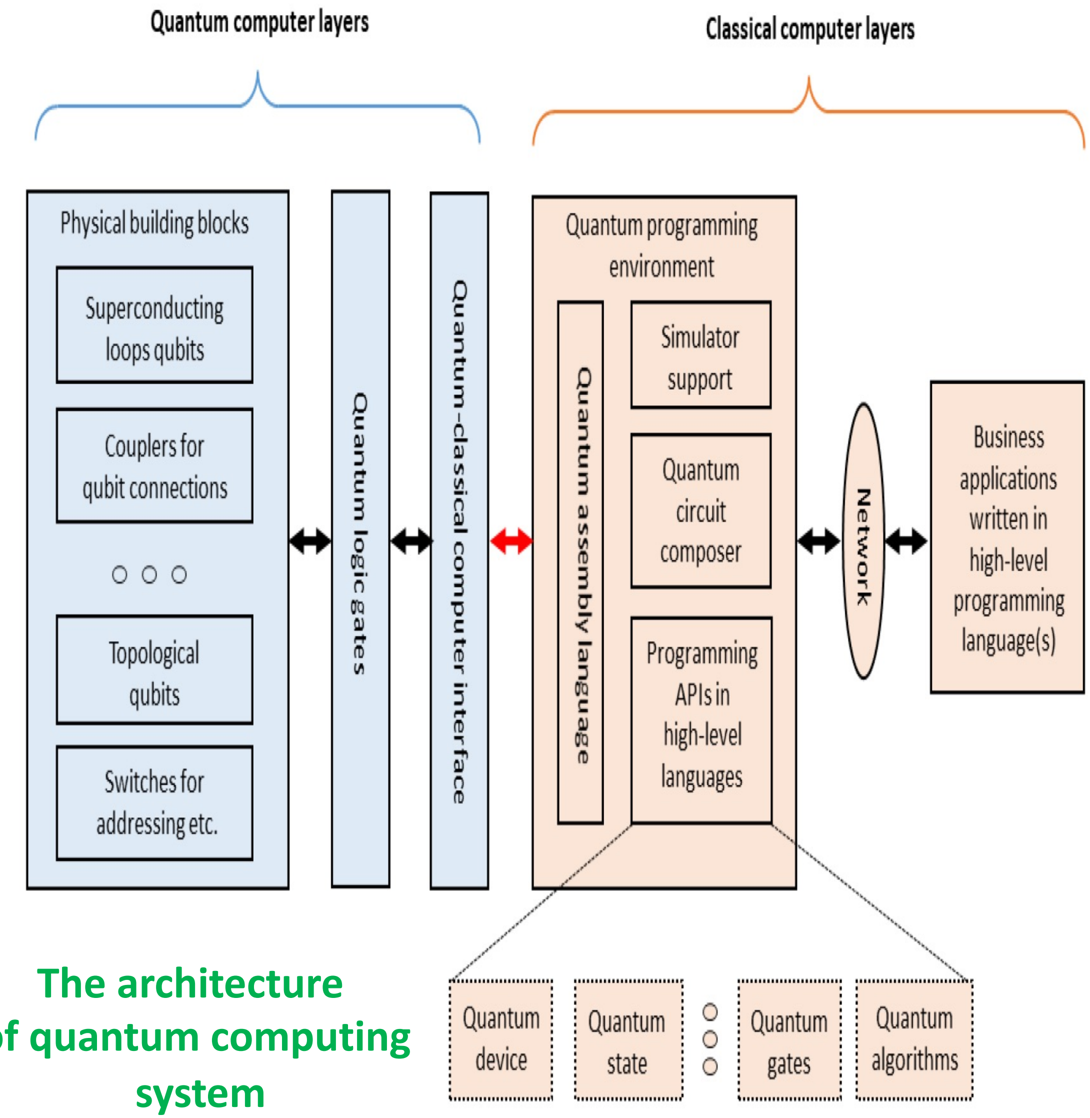
In this definition, we would like to highlight *three important issues in QSE*.
***First*, it is important to apply the "sound engineering principles“ to quantum software development.**
***Second*, the quantum software should be built "economically.“**
***Finally*, the quantum software should be "reliable“ and needs to work "efficiently" on quantum computers.**
Quantum software engineering can be regarded as a branch of systems engineering, which involves the development of large and complex quantum software systems.

V.V. Korenkov, A.G. Reshetnikov, S.V. Ulyanov, Quantum software engineering Pt 3: Quantum supremacy modelling. – M.: Kurs, 2021.



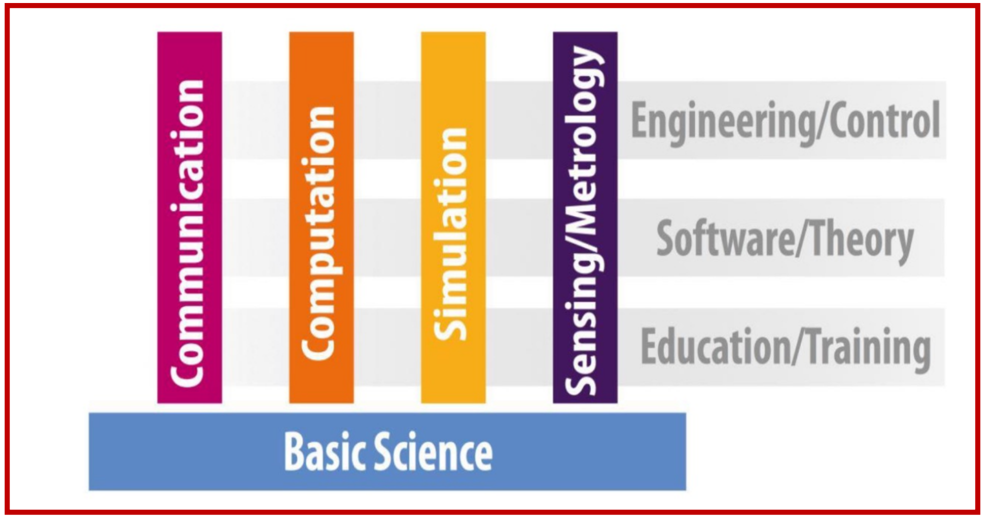
A Quantum Software lifecycle

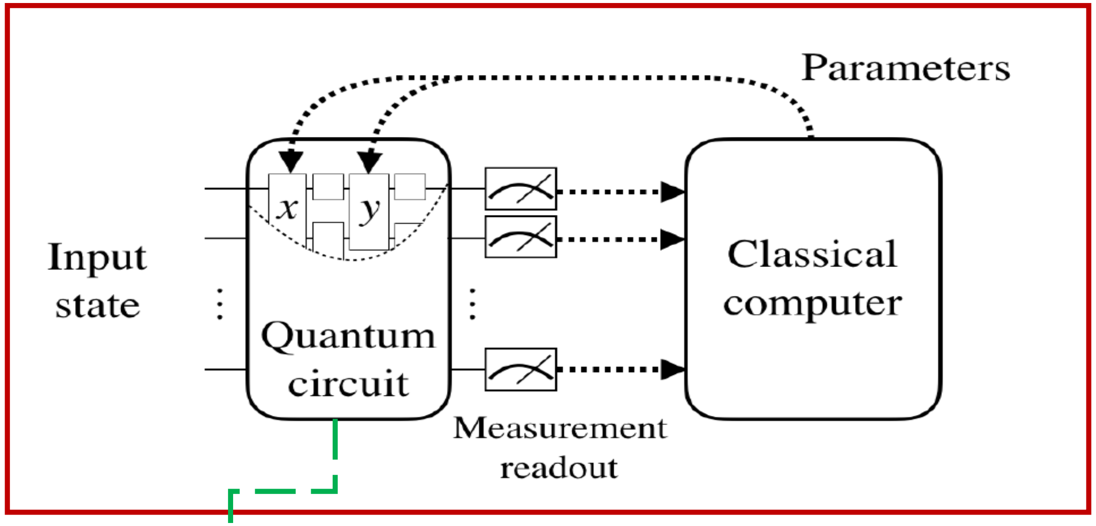
QSE embraces the coexistence of classical and quantum computing, and advocates the use of reengineering techniques to integrate new quantum algorithms with the existing classical Information systems. Reverse engineering techniques are also needed to parse and abstract quantum program information that is to be integrated into classical programs

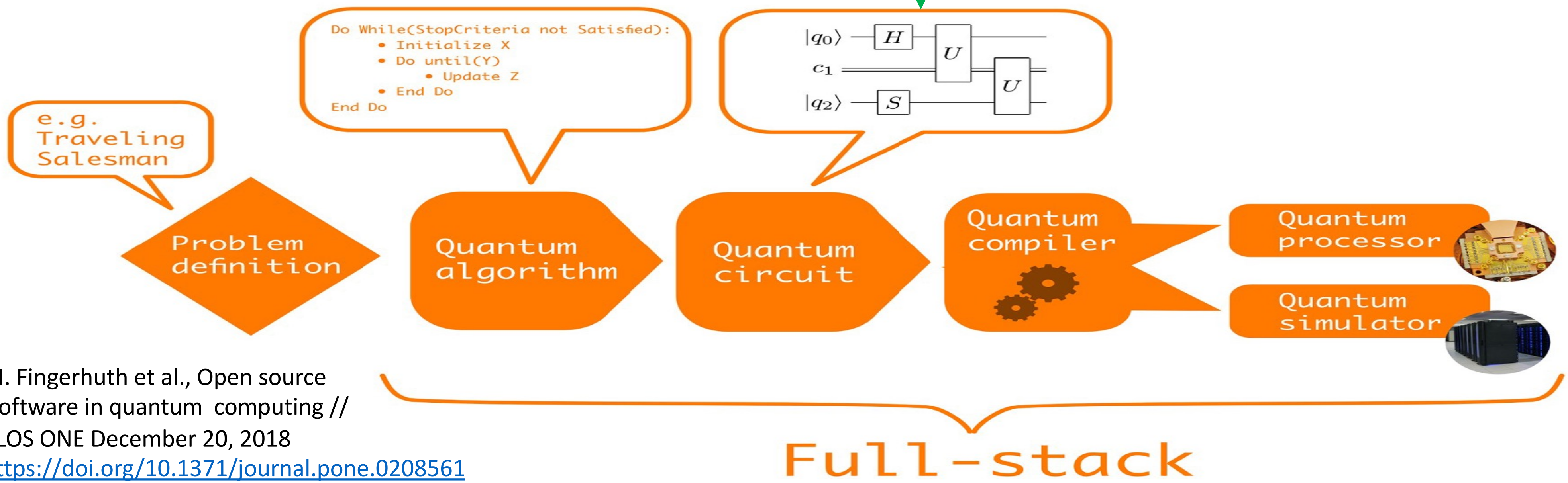


The architecture of quantum computing system

2. Quantum computational intelligence toolkit

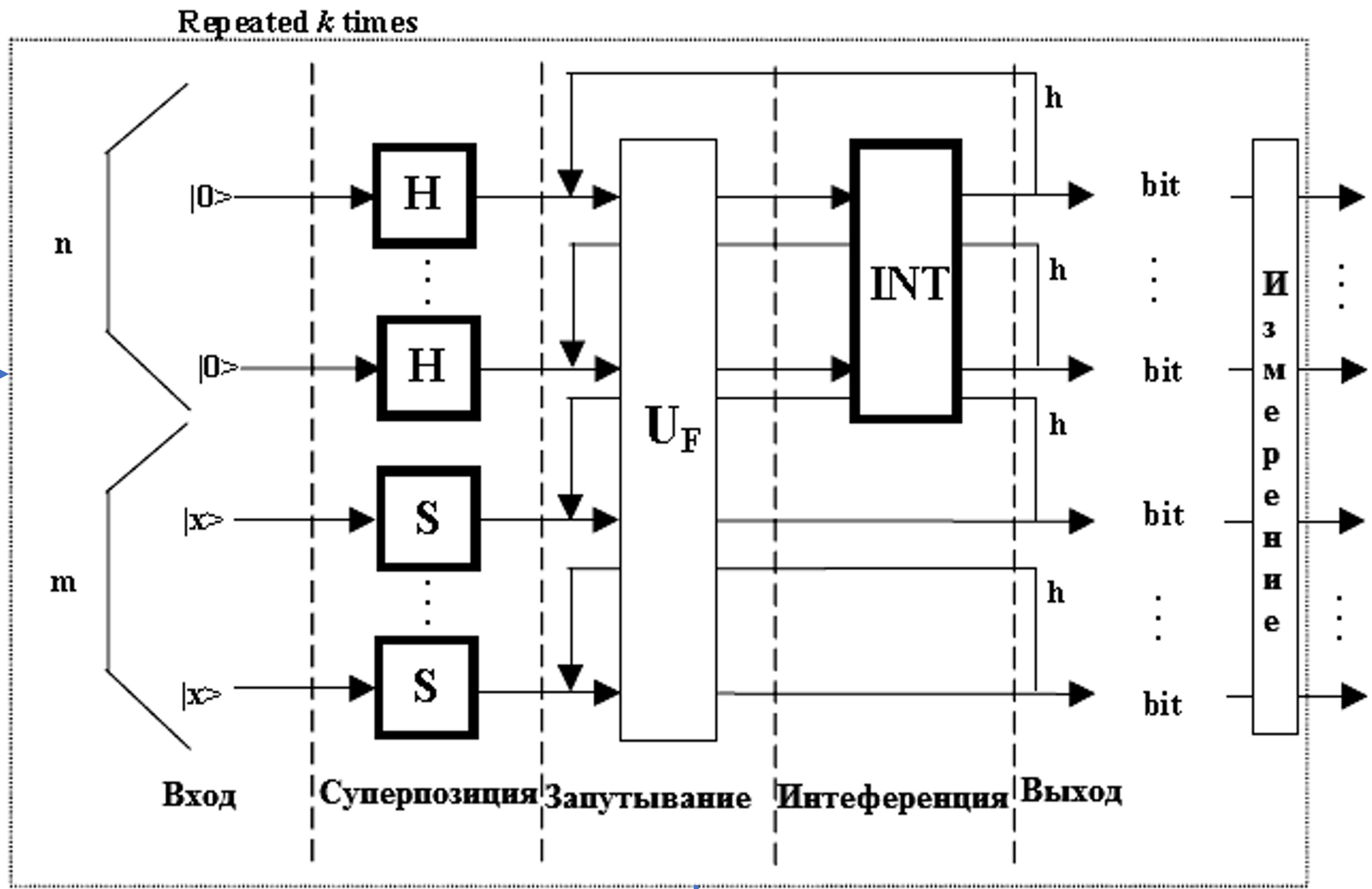






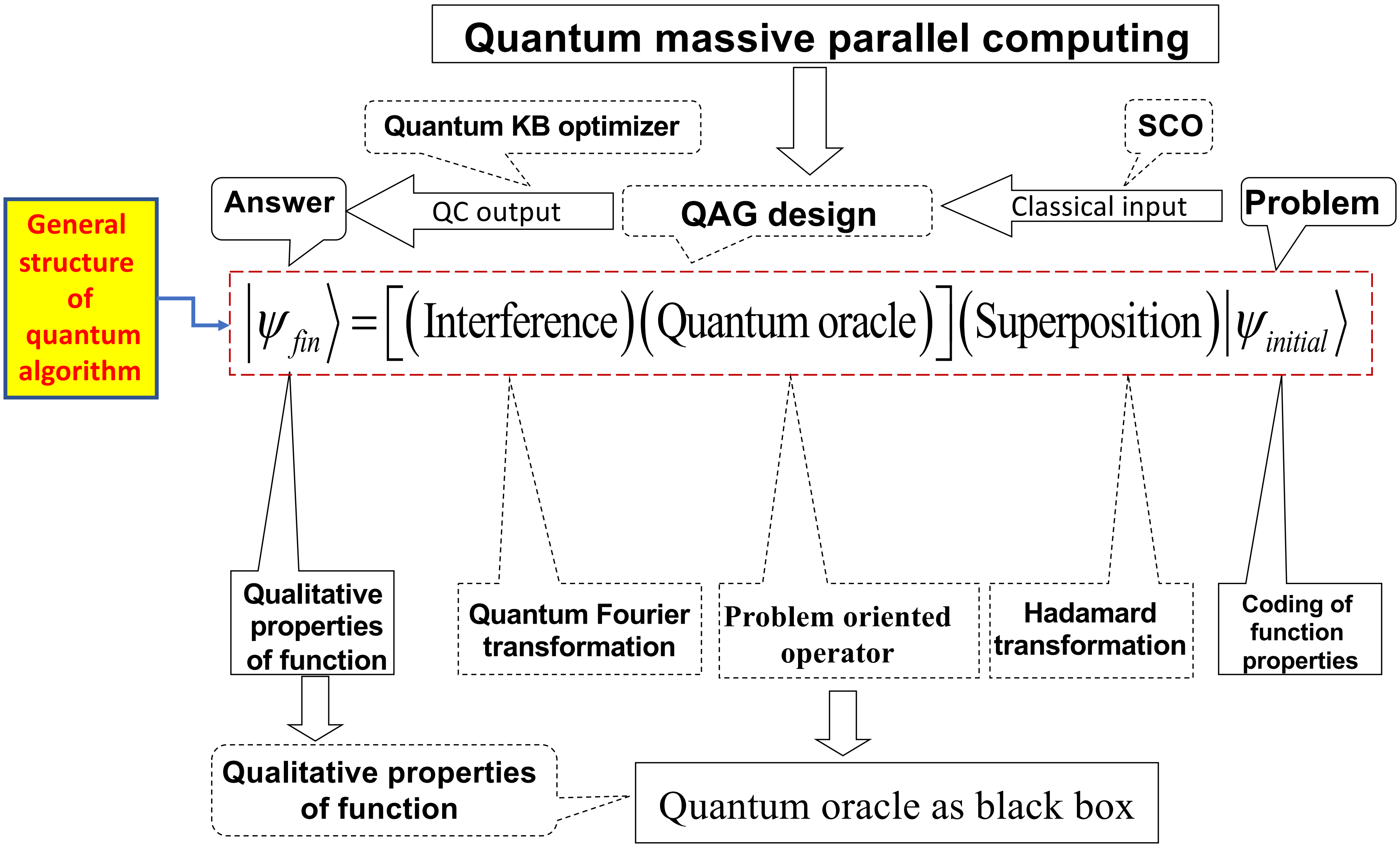
M. Fingerhuth et al., Open source software in quantum computing //
PLOS ONE December 20, 2018
https://doi.org/10.1371/journal.pone.0208561

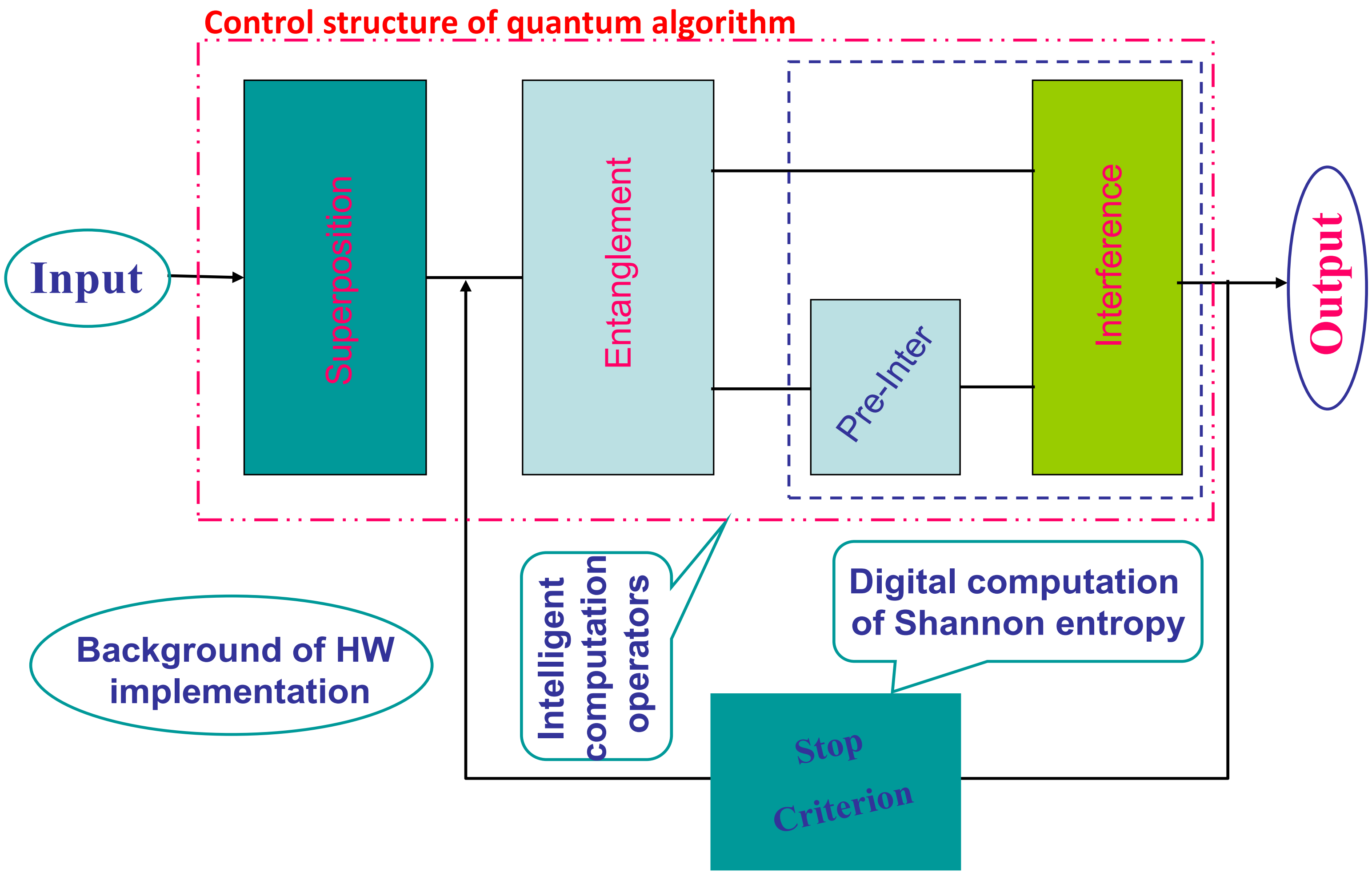
Quantum algorithmic gate-based computing



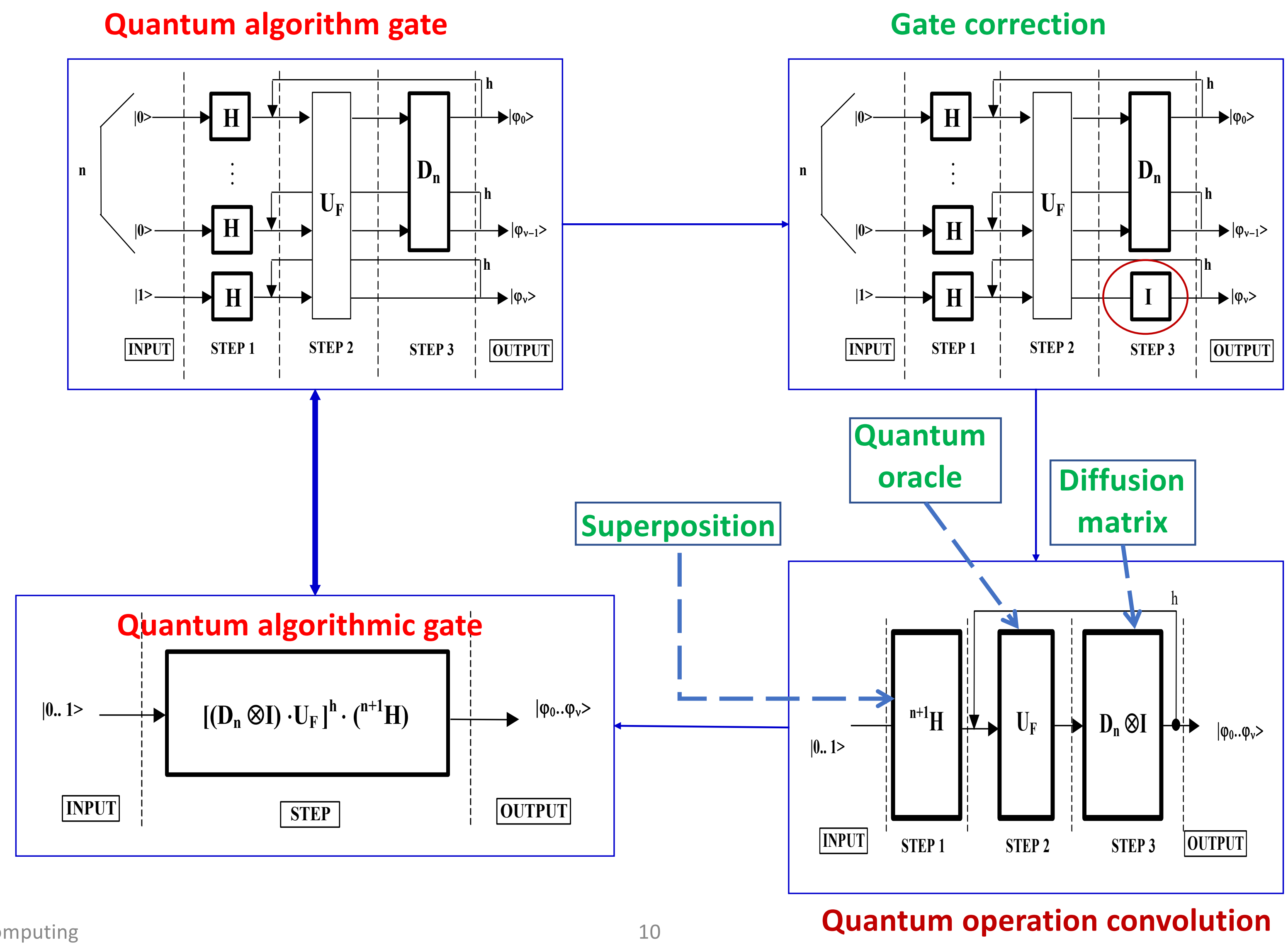
V.V. Korenkov, A.G. Reshetnikov, S.V. Ulyanov, Quantum software engineering. – M.: Kurs, 2021

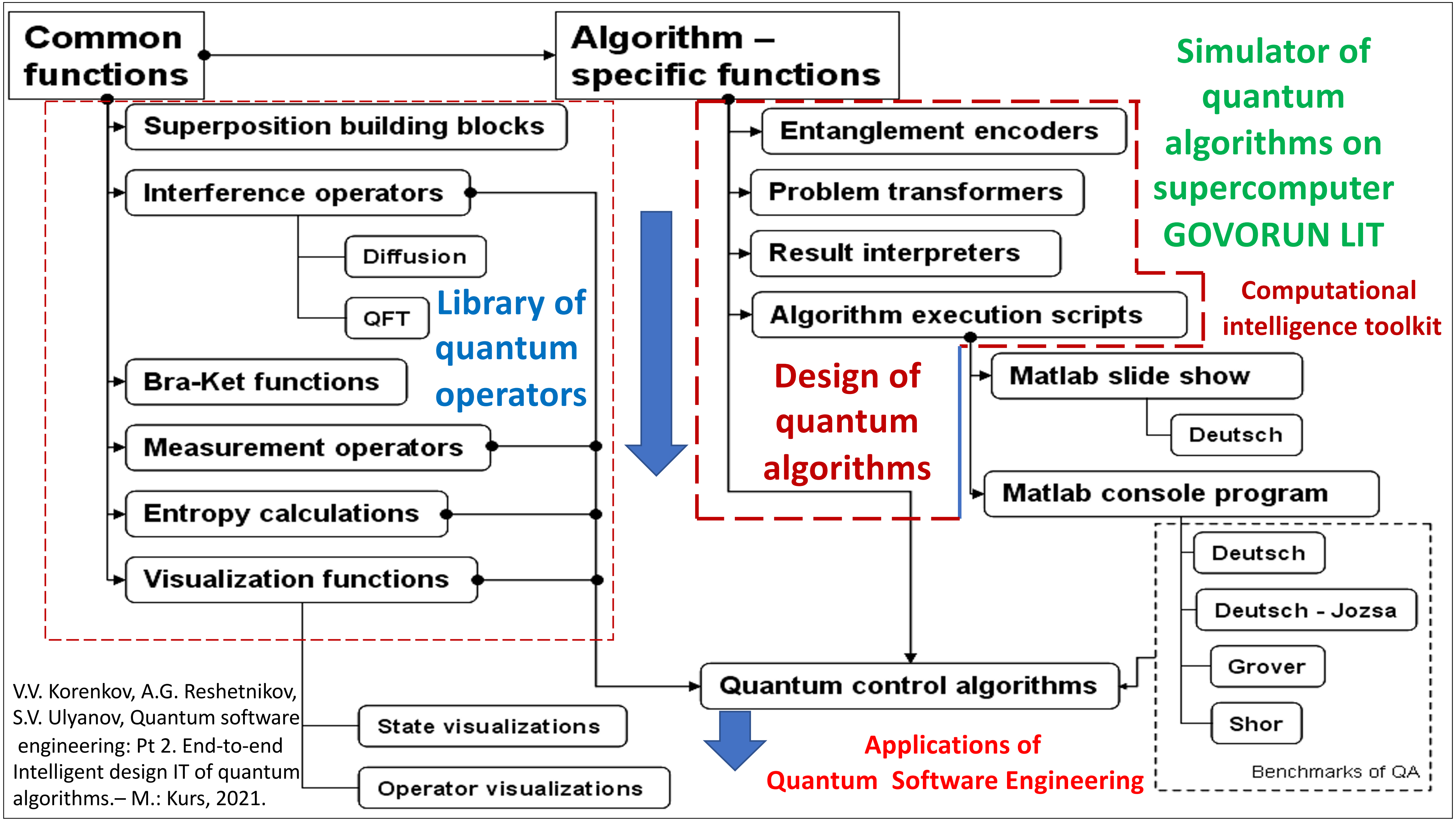
$$\text{КАЯ} = \left[\left(Int \otimes {}^{n} I \right) \cdot U_{F} \right]^{h+1} \cdot \left[{}^{n} H \otimes {}^{m} S \right]$$


Quantum massive parallel computing
Quantum KB optimizer
SCO
Answer
QC output
QAG design
Classical input
Problem
General structure of quantum algorithm
$|\psi_{fin}\rangle = [(\text{Interference})(\text{Quantum oracle})](\text{Superposition})|\psi_{initial}\rangle$
Qualitative properties of function
Quantum Fourier transformation
Problem oriented operator
Hadamard transformation
Coding of function properties
Qualitative properties of function
Quantum oracle as black box


Control structure of quantum algorithm
Input
Superposition
Entanglement
Pre-Inter
Interference
Output
Intelligent computation operators
Digital computation of Shannon entropy
Background of HW implementation
Stop Criterion

a


Quantum algorithm gate
Gate correction
n
|0>
|0>
|1>
H
H
H
U_F
D_n
I
h
|φ0>
|φv−1>
|φv>
INPUT
STEP 1
STEP 2
STEP 3
OUTPUT
Quantum oracle
Diffusion matrix
Superposition
Quantum algorithmic gate
|0.. 1>
[(D_n ⊗I) ·U_F]^h · (^{n+1}H)
|φ0..φv>
STEP
^{n+1}H
D_n ⊗I
Quantum operation convolution

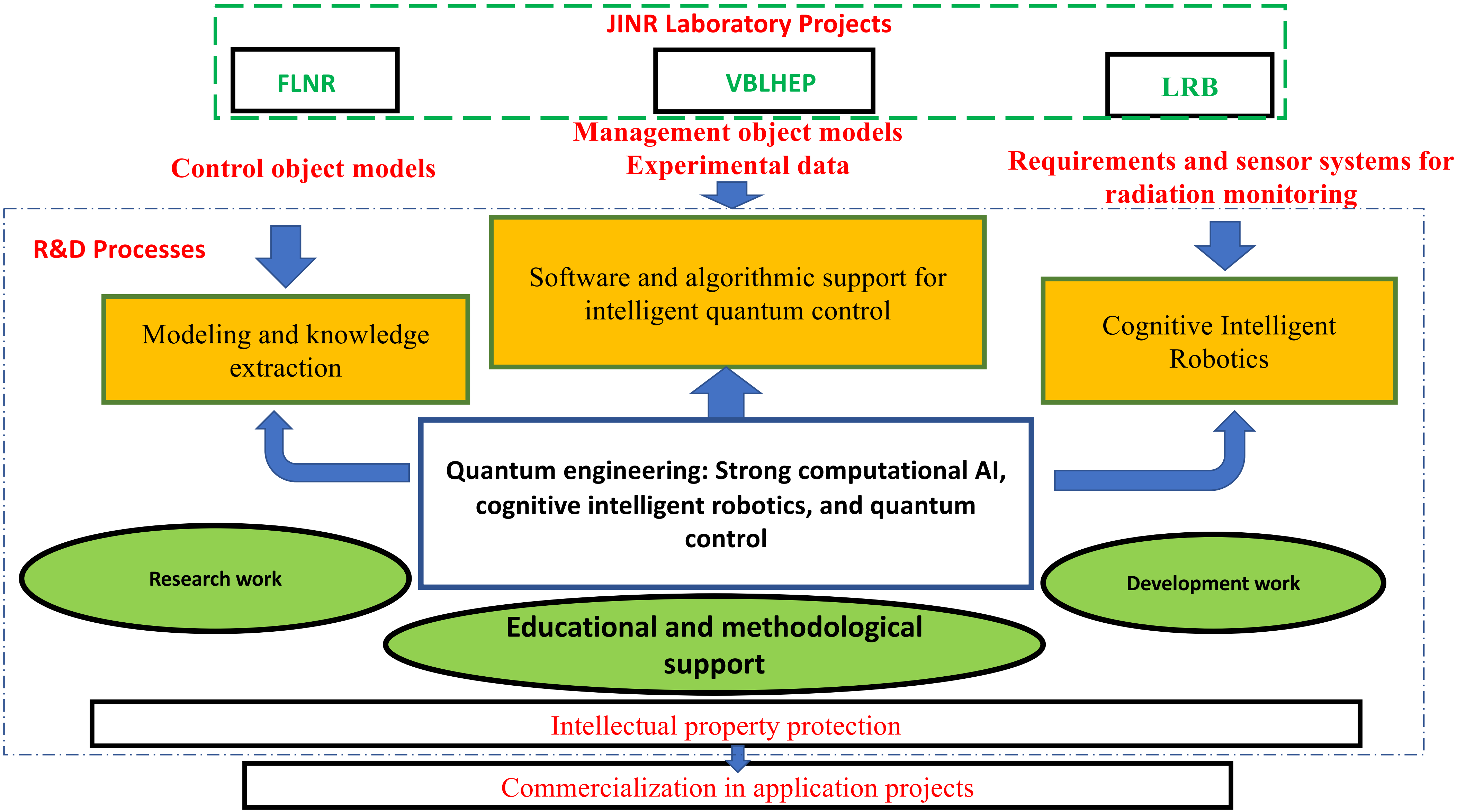

Common functions
Algorithm – specific functions
Superposition building blocks
Interference operators
Diffusion
QFT
Library of quantum operators
Bra-Ket functions
Measurement operators
Entropy calculations
Visualization functions
State visualizations
Operator visualizations
Entanglement encoders
Problem transformers
Result interpreters
Algorithm execution scripts
Simulator of quantum algorithms on supercomputer GOVORUN LIT
Computational intelligence toolkit
Design of quantum algorithms
Matlab slide show
Deutsch
Matlab console program
Deutsch
Deutsch - Jozsa
Grover
Shor
Benchmarks of QA
Quantum control algorithms
Applications of Quantum Software Engineering
V.V. Korenkov, A.G. Reshetnikov, S.V. Ulyanov, Quantum software engineering: Pt 2. End-to-end Intelligent design IT of quantum algorithms.– M.: Kurs, 2021.

3. Quantum Engineering LIT: JINR projects examples

Quantum computing in quantum robust control design

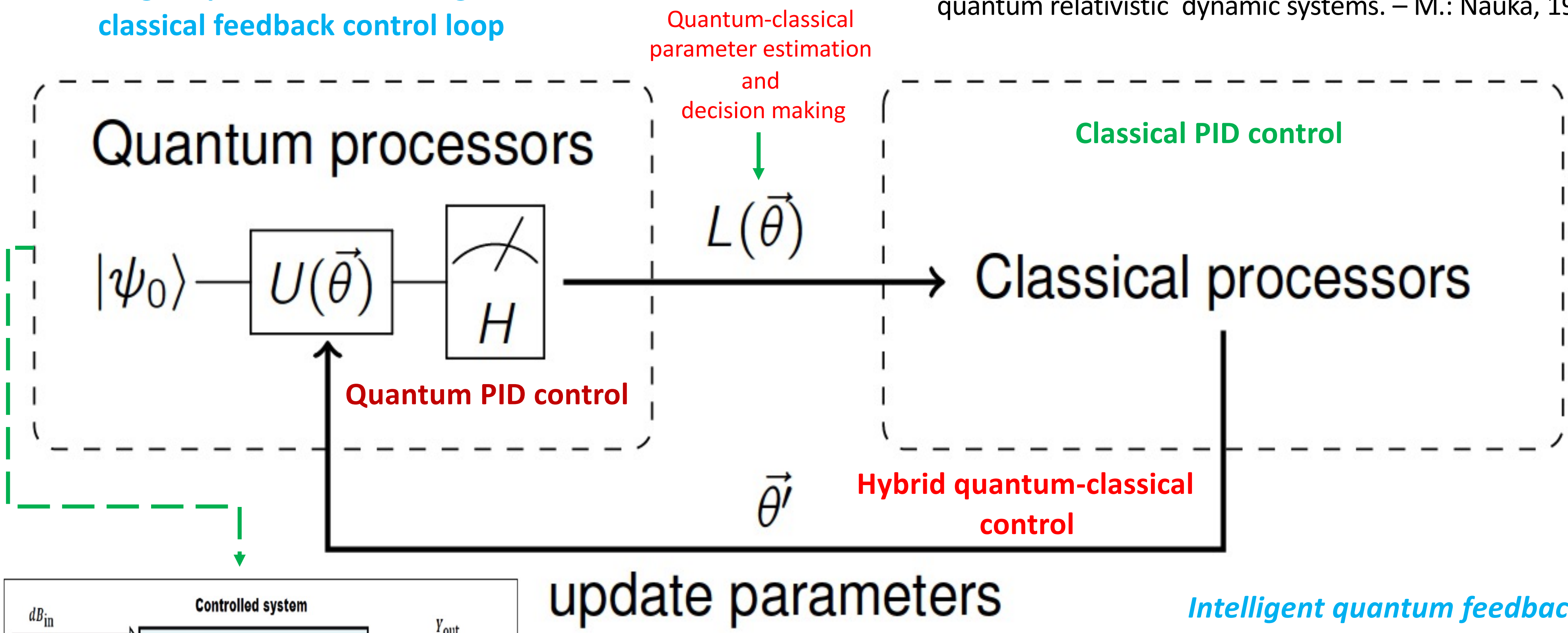
- ***Control of nitrogen consumption in superconducting-coil electromagnet***
- ***Control of high frequency station***
- ***Intelligent robotics control***

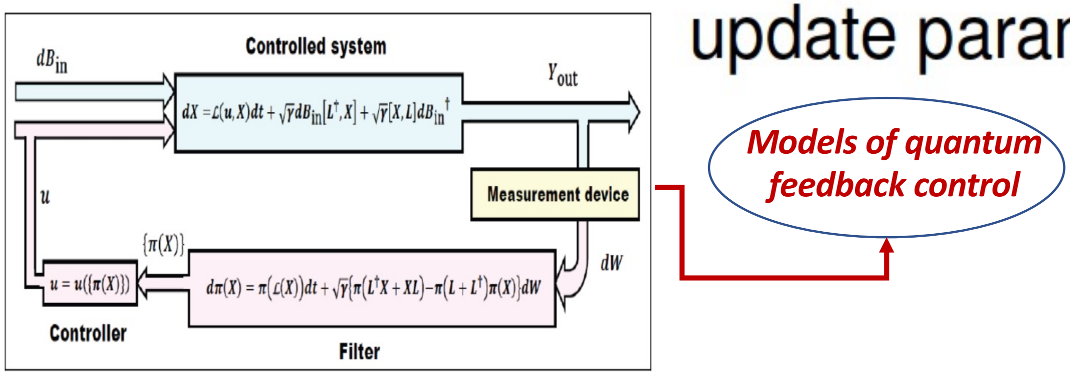
Quantum algorithms approach in the search structure of super-heavy elements


JINR Laboratory Projects
FLNR
VBLHEP
LRB
Management object models
Experimental data
Control object models
Requirements and sensor systems for radiation monitoring
R&D Processes
Software and algorithmic support for intelligent quantum control
Modeling and knowledge extraction
Cognitive Intelligent Robotics
Quantum engineering: Strong computational AI, cognitive intelligent robotics, and quantum control
Research work
Development work
Educational and methodological support
Intellectual property protection
Commercialization in application projects

Embedding of quantum control algorithm in classical feedback control loop

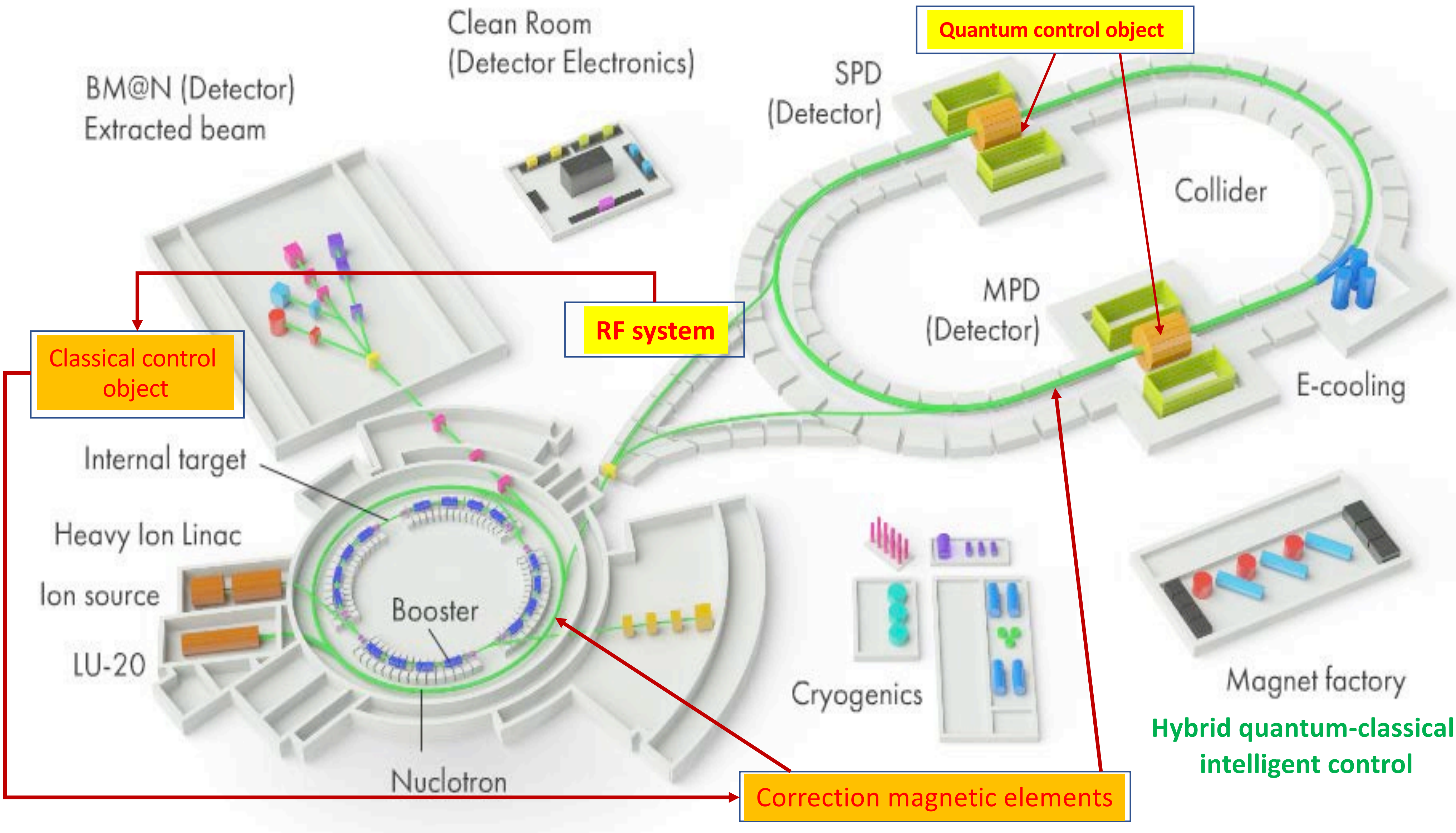
B.N. Petrov, I.I. Goldenblat, S.V. Ulyanov, Control problems of quantum relativistic dynamic systems. – M.: Nauka, 1982.





***Intelligent quantum feedback control*:**

S.V. Ulyanov, Quantum relativistic informatics: Unconventional logic of physical rigor and mathematical correctness of control object models. - LAP Acad. Publ., Germ.2014



Clean Room
(Detector Electronics)
BM@N (Detector)
Extracted beam
SPD
(Detector)
Quantum control object
Collider
MPD
(Detector)
RF system
Classical control object
E-cooling
Internal target
Heavy Ion Linac
Ion source
Booster
LU-20
Cryogenics
Magnet factory
Hybrid quantum-classical intelligent control
Nuclotron
Correction magnetic elements

Physical features of the control object and the physical process

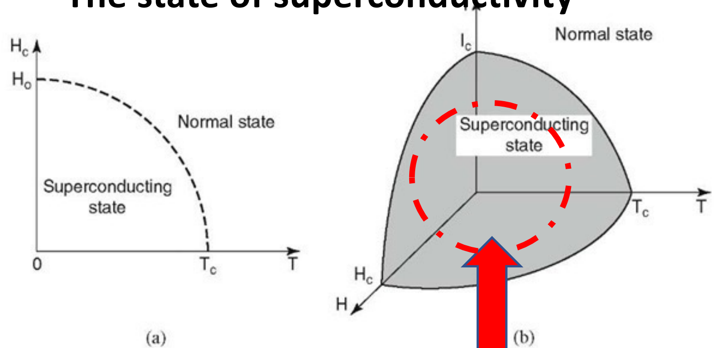
Features of an autonomous object

•Non-standard heat intakes
•Eddy currents in the core (heat the core)
•The dependence of the quality of the magnetic field on the quality of cooling
•Flashing of the wall and uneven cooling in the connecting nodes



The control task is to maintain the state of superconductivity

The state of superconductivity



The point of equilibrium in space and the permissible range of changes in current, temperature, and magnetic field

Features of the group of magnetic elements

•Different eddy currents in the core
•Minor differences in magnets elements

The principle of intelligent control: **Compensation of the indeterminate and inaccurate parameters of the magnetic element existing in a real object through the use of soft and quantum computing technologies**

Intelligent robotic quantum control

Intelligent robotics based on quantum fuzzy inference

- Structure of self-organized intelligent control system
- Robotic redundant 7 DoF manipulator
- Autonomous and swarm robots with information exchange (video)

Robust Intelligent Control in Unpredicted Control Situations Relative to Quantum Knowledge: KB Self-organization Phenomena based on Quantum Fuzzy Inference

- **Examples of simulation and benchmarks demo**

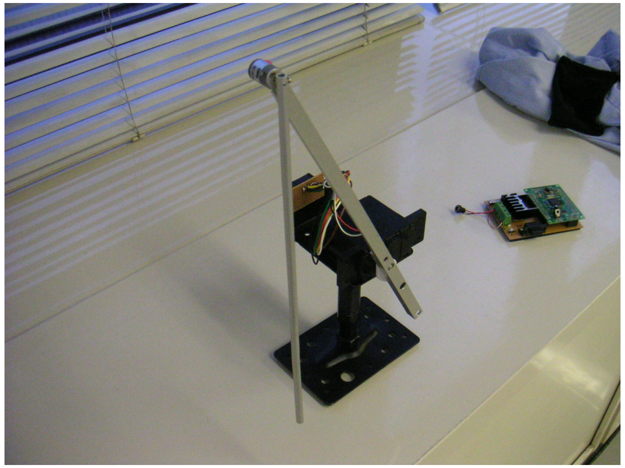
(cart – pole dynamic system)

Inverted Pendulum

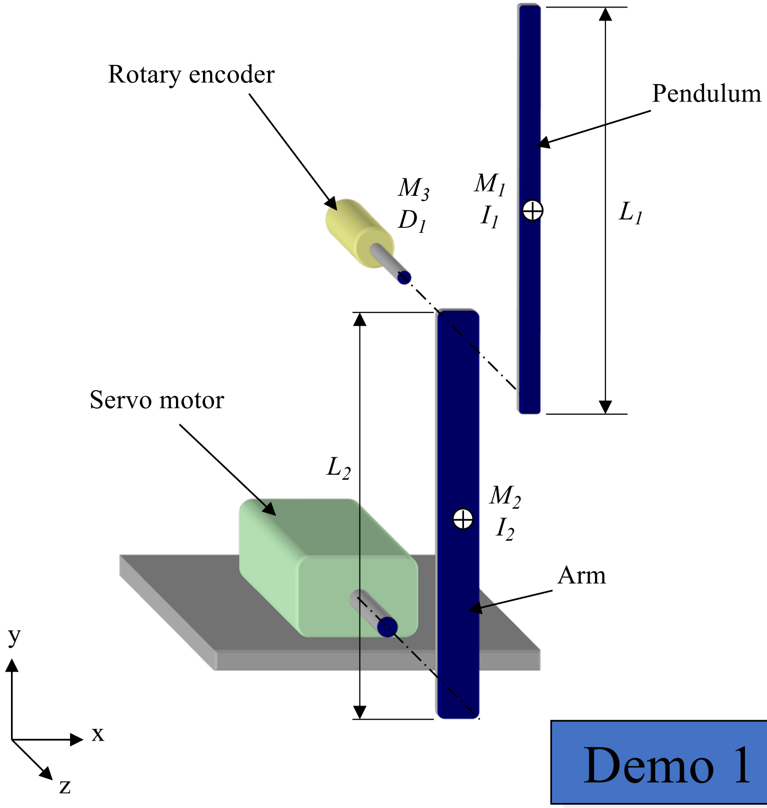
Intelligent control of the pendulum based on the physical measurements

Without The knowledge of his mathematical model

Inverted pendulum hardware model



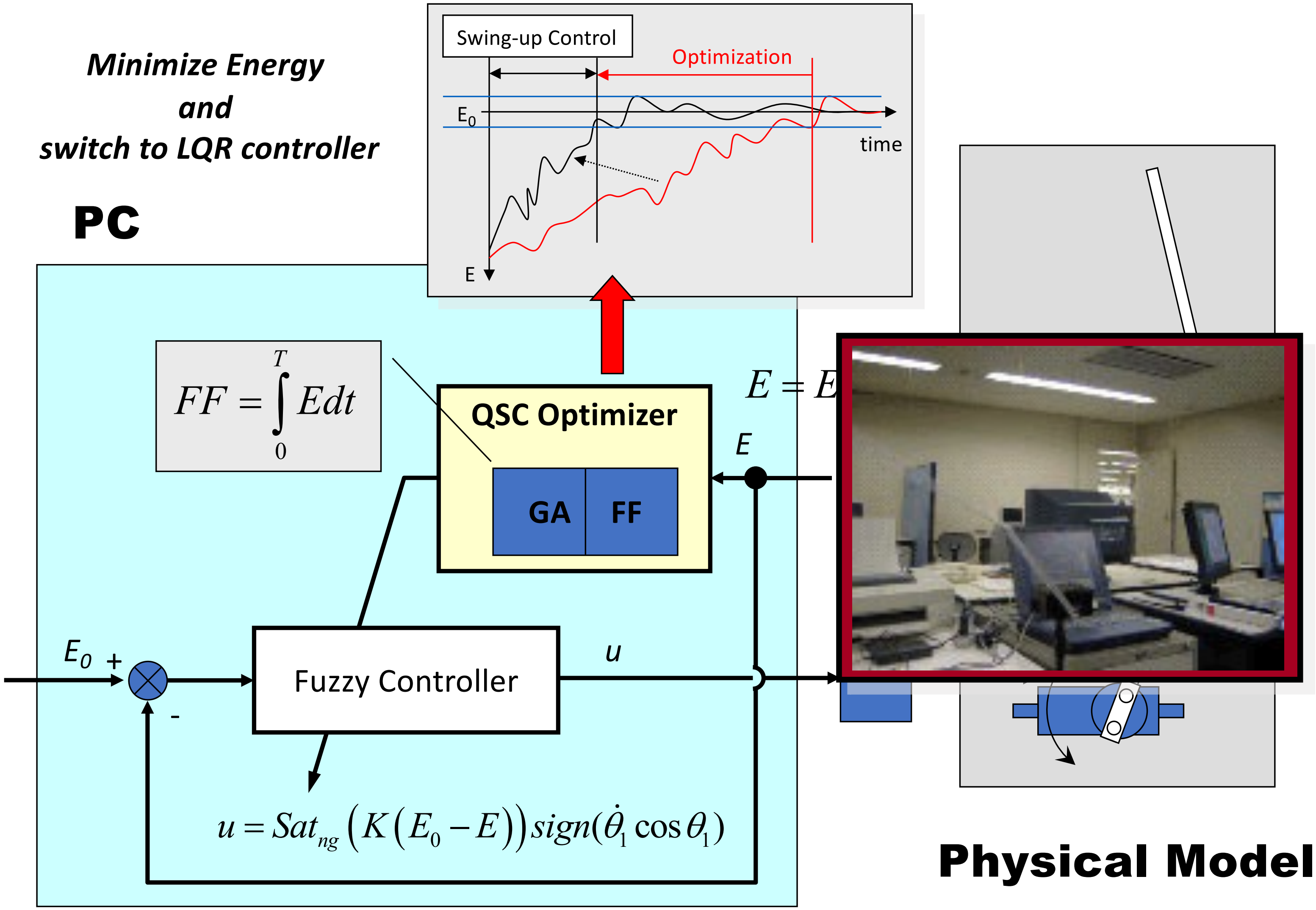
Pendulum	length	L_1	0.29	m
	mass	M_1	1.23E-2	kg
	momentum inertia	I_1	8.62E-5	kgm^2
Arm	length	L_2	0.23	m
	mass	M_2	1.12E-2	kg
	momentum inertia	I_2	4.93E-5	kgm^2
Rotary encoder	mass	M_3	1.00E-2	kg
	damping	D_1	5.00E-5	Ns/m



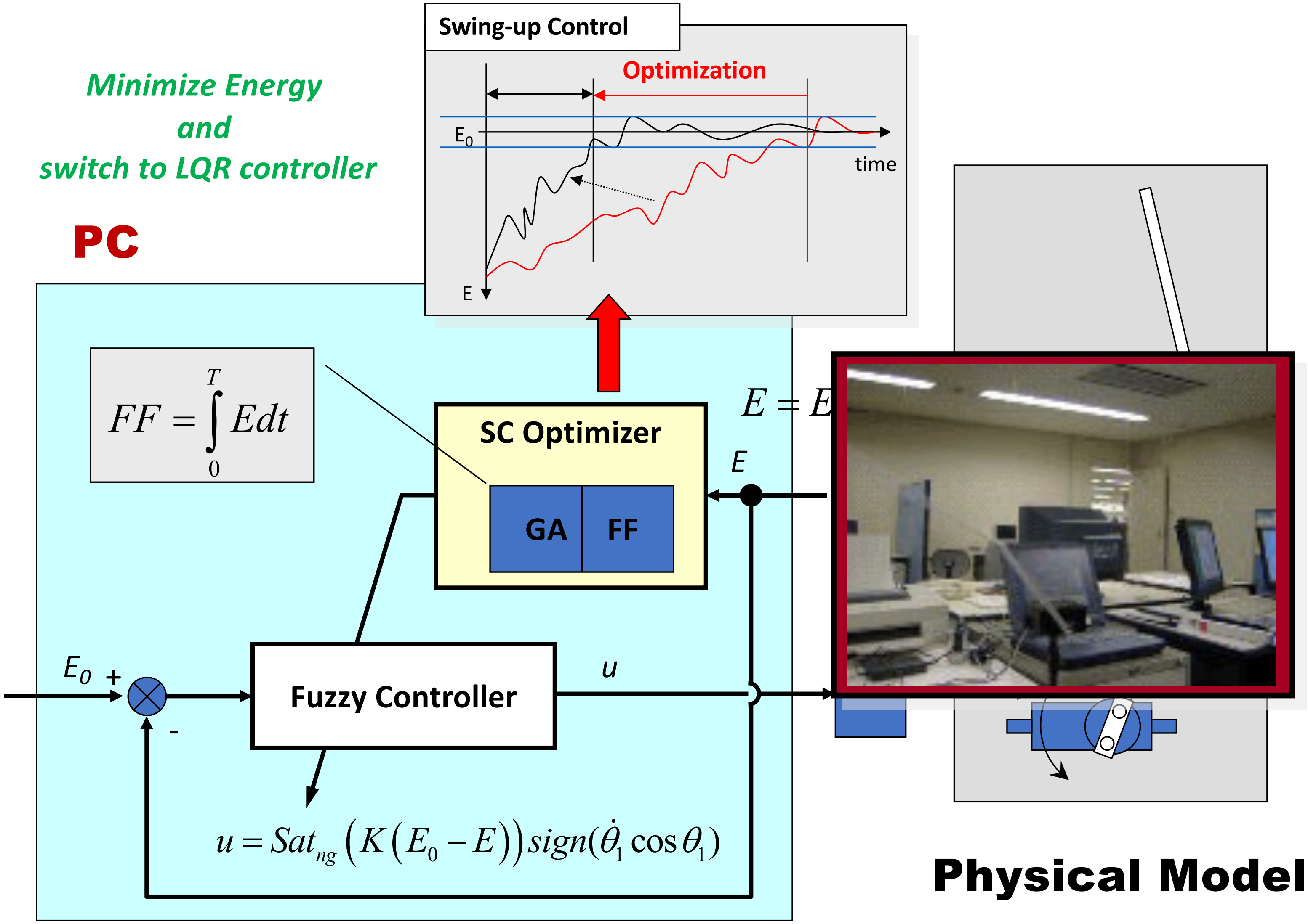
Demo 1

Demo 2

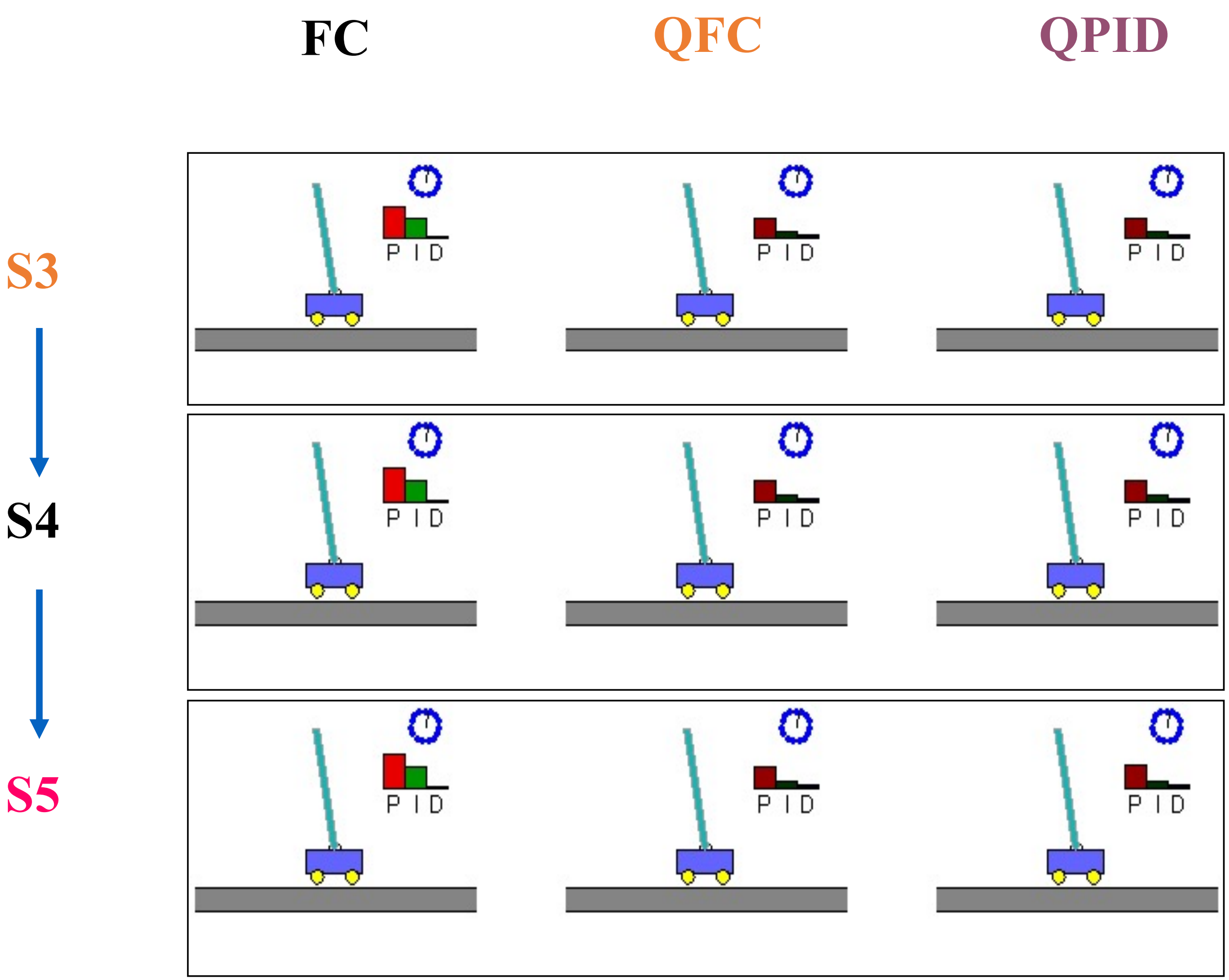
Direct Swing-Up Optimization by QSCOptimizer



Direct Swing-Up Optimization by SCOptimizer

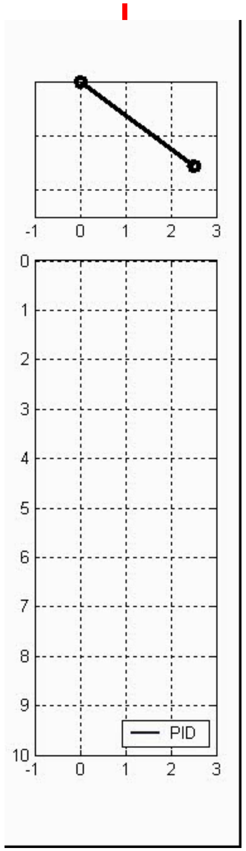


100 frames sample

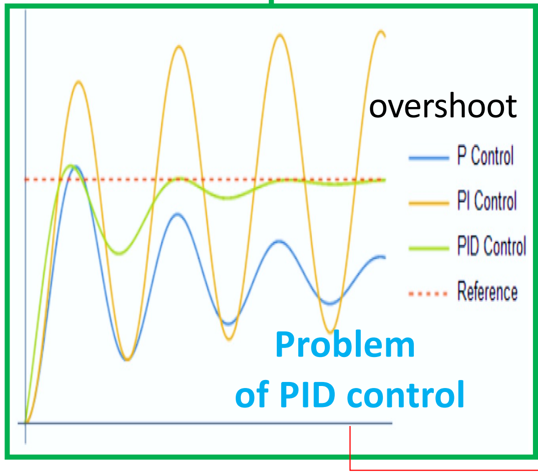


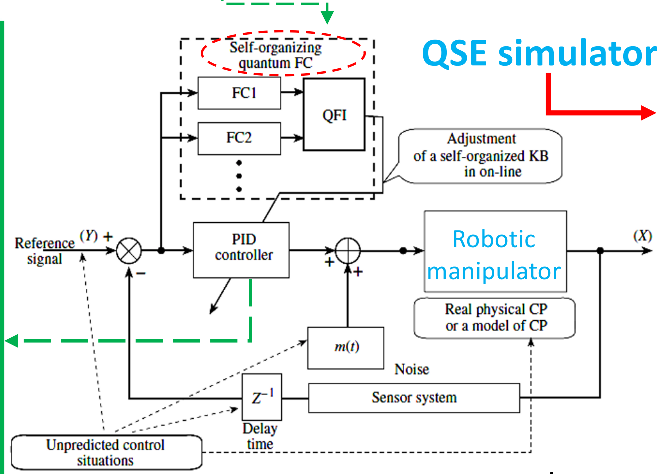
Structure of self-organized intelligent control system

Video

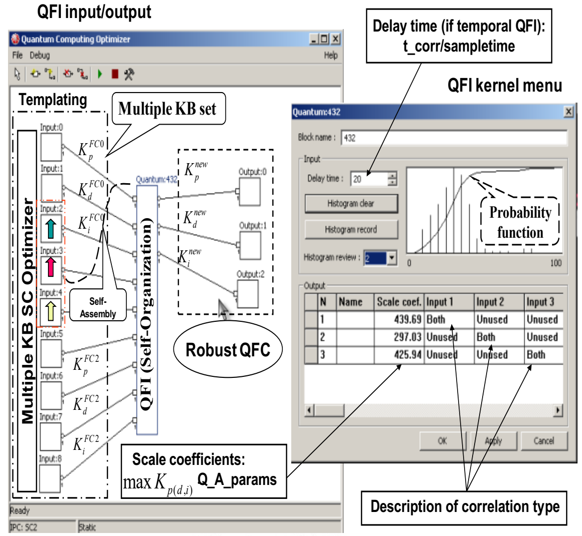


Robust control of pendulum under random excitation

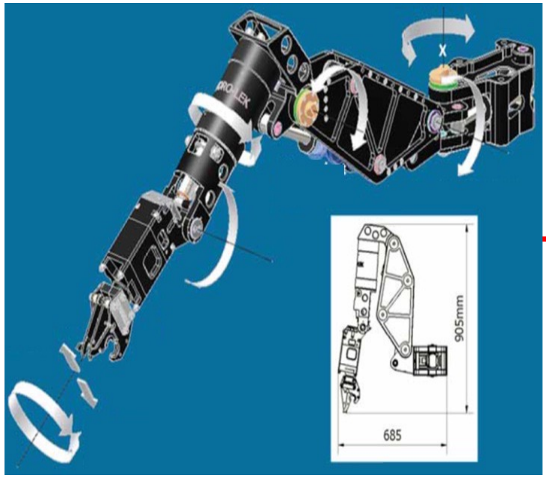




QSE simulator



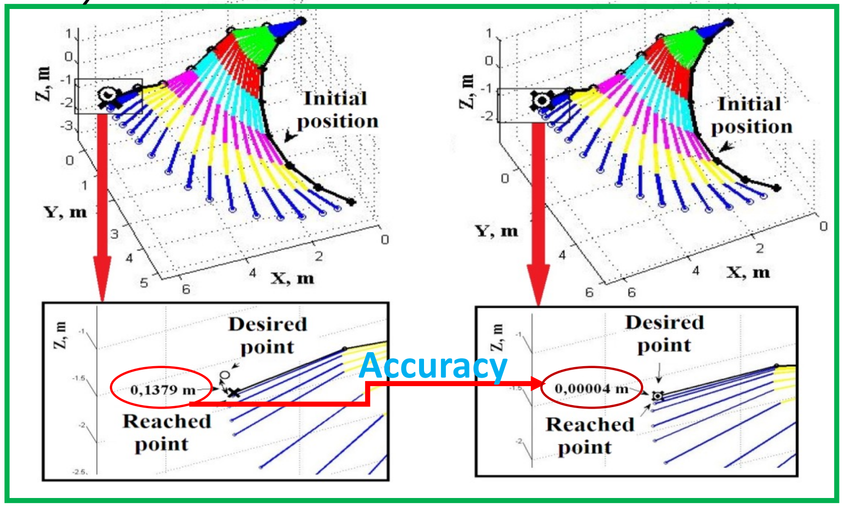
Intractable conventional control problem



7 degree of freedom redundant manipulator

QSE supremacy
In robotics control

Fuzzy PID control



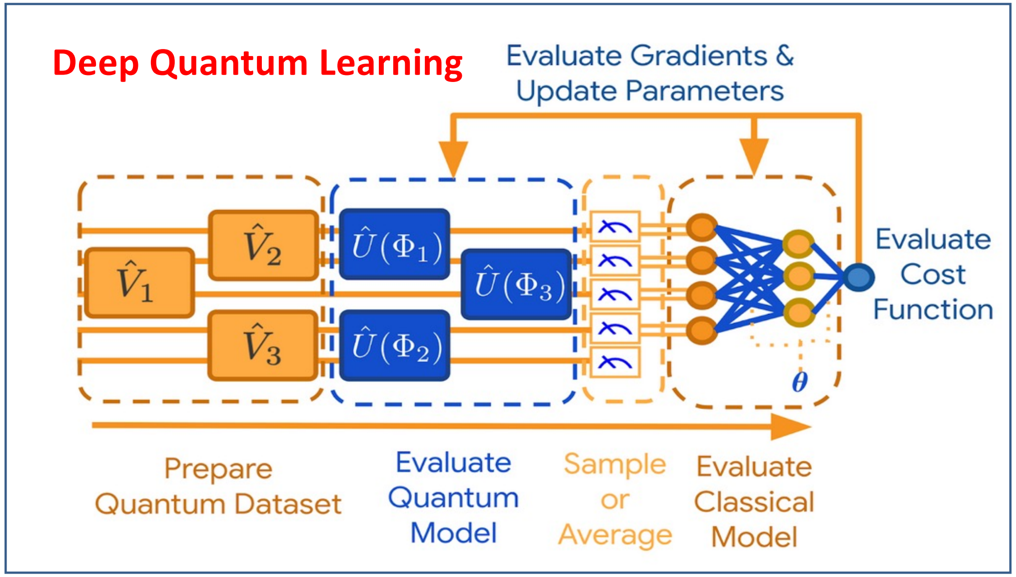
Quantum PID control

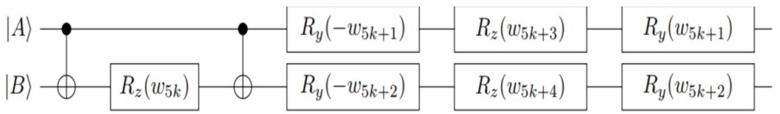
V.V. Korenkov; A.G. Reshetnikov; S.V. Ulyanov, Quantum Software Engineering Supremacy in Intelligent Robotics // Published in: 2020 International Scientific and Technical Conference Modern Computer Network Technologies (MoNeTeC)

[redacted]

Quantum intelligent control

- **Quantum deep learning**
- **Quantum control of relativistic physical objects**

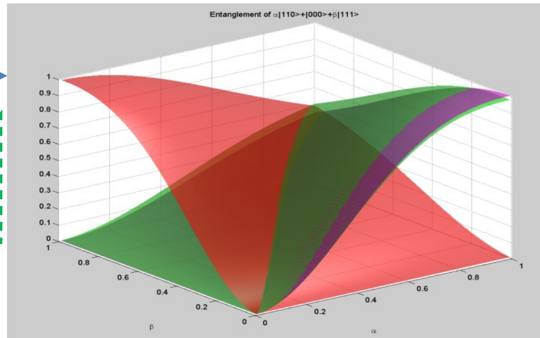




This the quantum circuit for the gate decomposition of a single time chunk of the entanglement witness.

The 2 qubit operations are CNOT gates, *R* is a rotation about a designated axis on the Bloch sphere, and the *w* values are functions of the system parameters K.

Figure shows entanglement of $|110\rangle + \beta|111\rangle + |000\rangle$ as a function of both α and β, and compared with the three-way "tangle" agreement is quite good. The red surface shows the pairwise entanglement between qubits *A* and B, the green; 3-way entanglement among A, B, and C; the magenta is the (analytically calculated) 3-tangle.



J.E. Steck, E. C. Behrman, and N. Thompson,
Machine Learning applied to Programming Quantum Computers // Conference paper, 2019.
https://www.researchgate.net/publication/330199278

Lagrangian quantum deep learning

The density matrix, ρ, of a quantum system as a function of time obeys the Schrödinger equation

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[H,\rho]$$

and has the formal solution as $\rho = \exp(iLt)\,\rho(t_0)$. The time evolution equation for the density matrix maps the initial state ρ(t0) (input data for the quantum computer) to the final state $\rho(t_f)$ (output calculated result). Parameters in the system Hamiltonian *H* are physical interactions and fields in quantum hardware and can be adjusted experimentally as functions of time. "Programming" this quantum computer involves finding the parameters using machine learning that yield the desired computation. Thus, we can train the system to evolve in time initial (input) to target final (output) states; yielding a quantum system that accurately approximates a chosen function, such as: logic gates, benchmark classification problems, or, since the time evolution is quantum mechanical, a quantum function like entanglement.

The learning rule for the quantum system based on dynamic backpropagation is derived as follows. Given an input (initial density matrix), ρ_0, and a target output, *d* (a "training pair"), we develop a weight update rule based on gradient descent to adjust the system parameters, i.e., train the system "weights", to reduce the squared error between the target, *d*, and the output, Output. While minimizing the squared error, the system's density matrix, ρ(t), is constrained to satisfy the Schrödinger equation for all time in the interval (t_0, t_f). We define a Lagrangian, *L*, to be minimized, as

$$L = \tfrac{1}{2}[d - < O(t_f) >]^2 + \int_{t_0}^{t_f} \lambda^+(t)\left(\frac{\partial\rho}{\partial t} + \frac{i}{\hbar}[H,\rho]\right)\gamma(t)\ \ dt$$

where the Lagrange multiplier vectors are $\lambda^{+}(t)$ and γ(t) (row and column, respectively), and *O* is an output measure (or some function of a measure), which is chosen for the particular problem under consideration. As an example, for our entanglement witness application, we defined the output as:

$$\langle O(t_f)\rangle = tr[\rho(t_f)O] = \textstyle\sum_i p_i\langle\psi_i(t_f)|O|\psi_i(t_f)\rangle$$

where *tr* stands for the trace of the matrix, and where the density matrix is represented in terms of the chosen basis as $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. We take the first variation of *L* with respect to ρ, set it equal to zero, then integrate by parts to give the following equation which can be used to calculate the vector elements of the Lagrange multipliers ("error deltas" in neural network terminology) that will be used in the learning rule:

$$\gamma_i\frac{\partial\gamma_j}{\partial t} + \frac{\partial\lambda_i}{\partial t}\gamma_j - \frac{i}{\hbar}\sum_k \lambda_k H_{ki}\gamma_j + \frac{i}{\hbar}\sum_k \lambda_i H_{jk}\gamma_k = 0$$

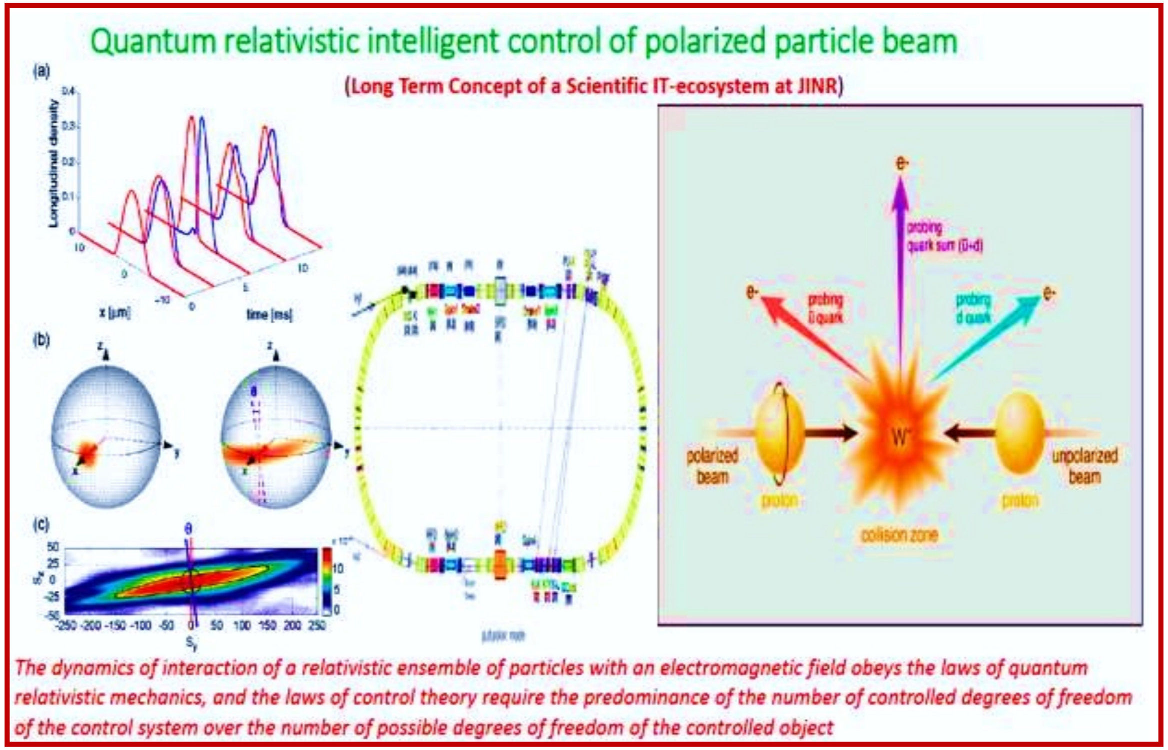
which is solved backward in time, with the boundary conditions at the final time t_f given by

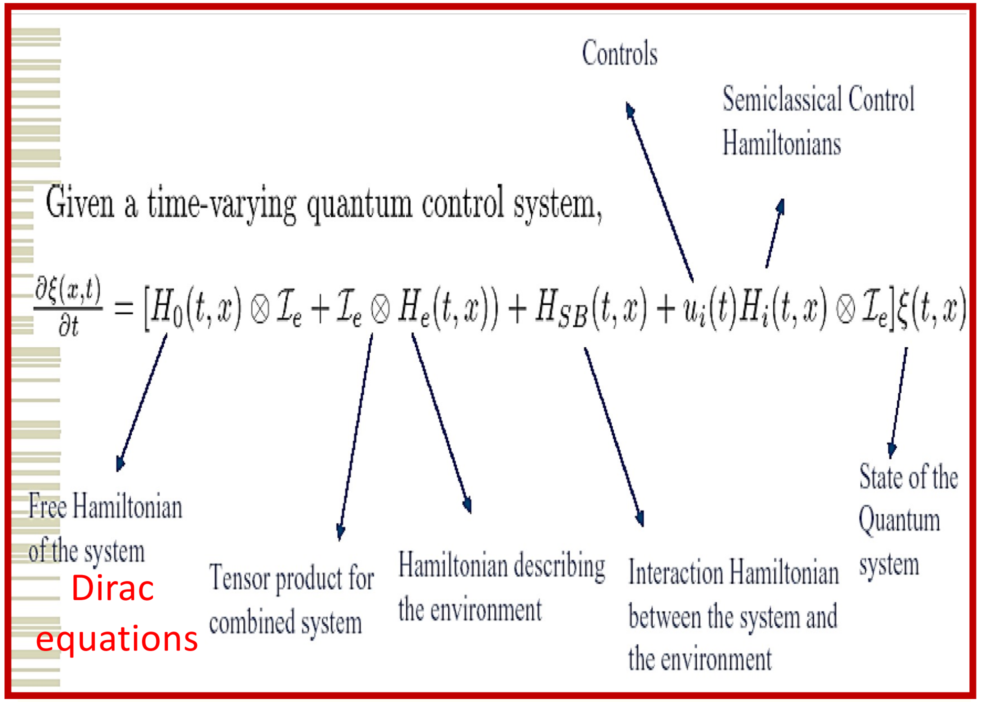
$$-\left[d - \langle O(t_f)\rangle\right]O_{ji} + \lambda_i(t_f)\gamma_j(t_f) = 0.$$

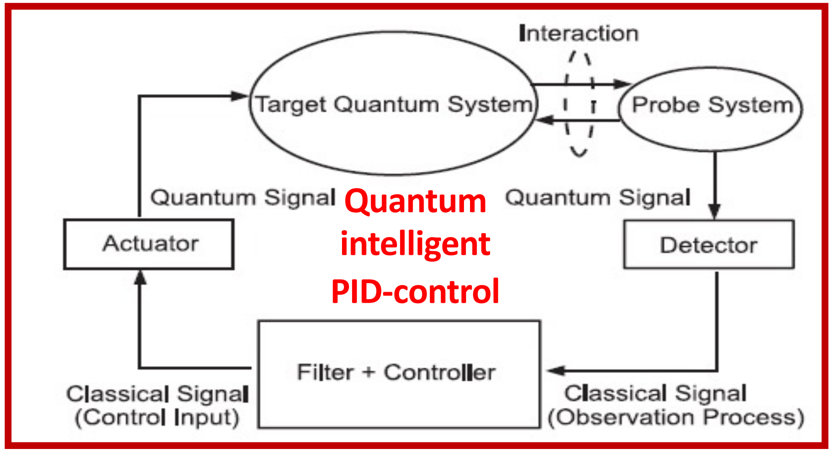
The gradient descent rule to minimize *L* with respect to *w* is $w_{new} = w_{old} - \eta\frac{\partial L}{\partial w}$ or each "weight" parameter *w*, where η is the learning rate, and where the derivative is given by

$$\frac{\partial L}{\partial w} = \frac{i}{\hbar}\int_0^{t_f}\lambda^+(t)\left[\frac{\partial H}{\partial w},\rho\right]\gamma(t)dt \ = \frac{i}{\hbar}\int_0^{t_f}\sum_{ijk}\left(\lambda_i(t)\frac{\partial H}{\partial w}\rho_{kj}\gamma_j - \lambda_i(t)\rho_{ik}\frac{\partial H_{kj}}{\partial w}\gamma_j\right)dt$$

The above technique, since it uses the density matrix, is applicable to any state of the quantum system, pure or mixed.

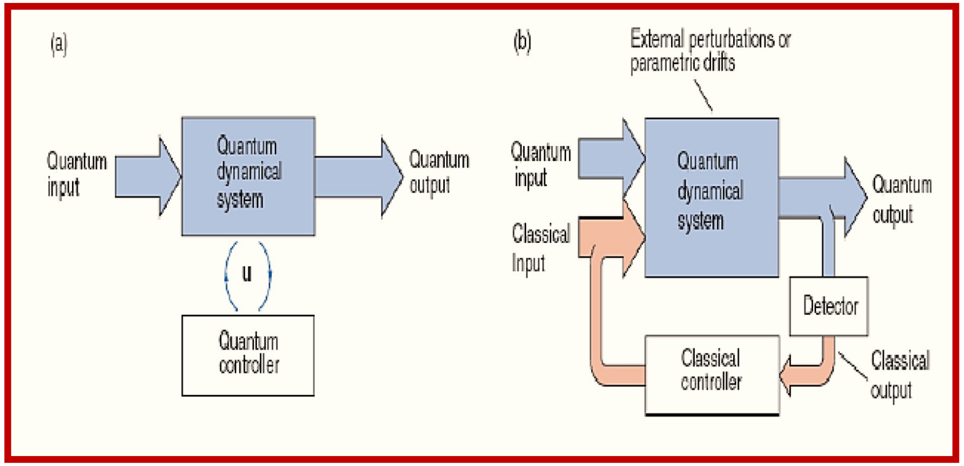






Quantum non-demolition feedback control of quantum object

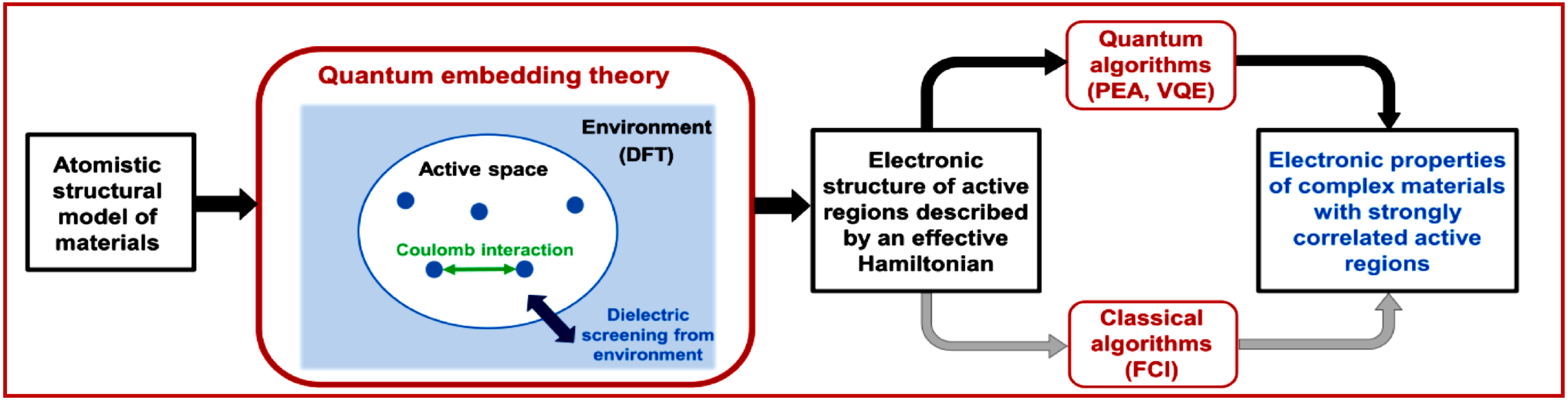
Quantum relativistic Informatics toolkit



Quantum simulation of super-heavy elements of Mendeleev's table:

Quantum gate based approach

General strategy for quantum simulations of materials using quantum embedding



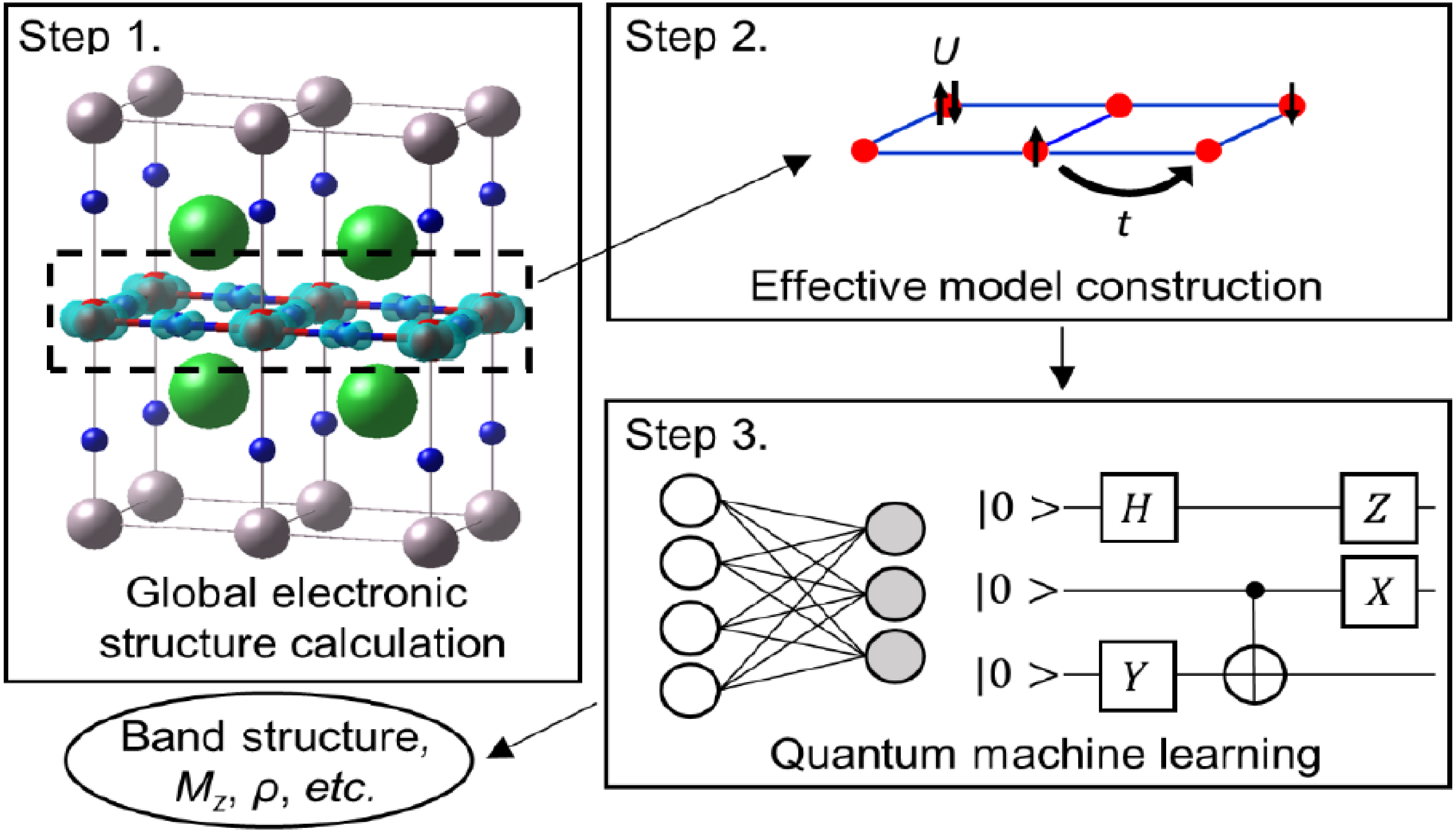
Quantum simulator

Example of effective application in quantum chemistry

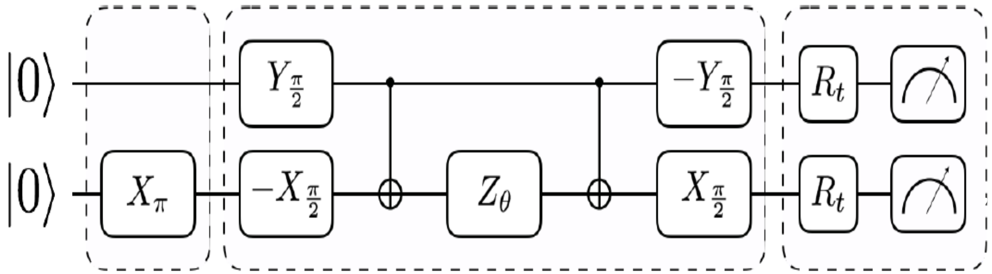
Quantum simulator

Example of effective application in quantum chemistry

Workflow for calculation of materials properties using quantum algorithm for many-body problems of inorganic systems



The quantum circuit used in VQE to estimate the ground state energy for molecular hydrogen in the minimal basis

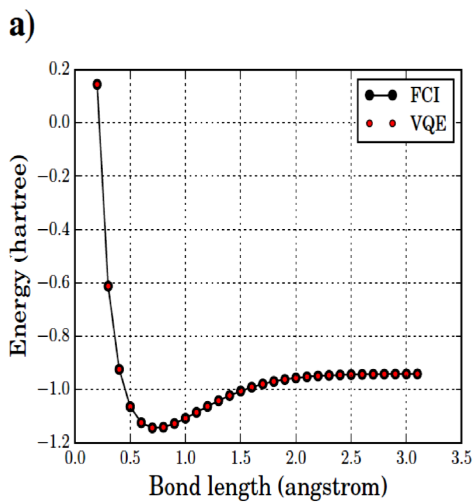


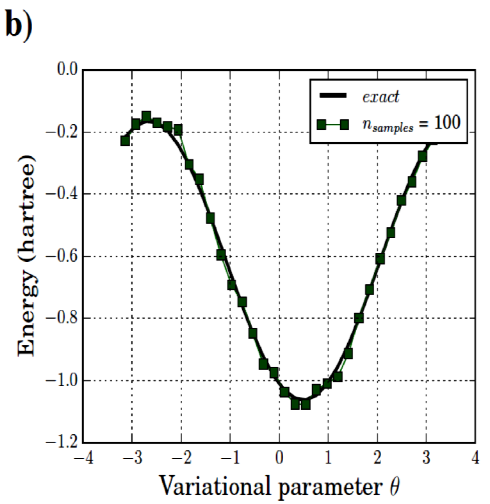
1. Prepare Hartree-Fock (mean-field) reference state.

2. Implement unitary coupled-cluster (UCC) ansatz.

3. Apply necessary post-rotations for energy estimation.

VQE simulation results for molecular hydrogen in the minimal basis (STO-6G)

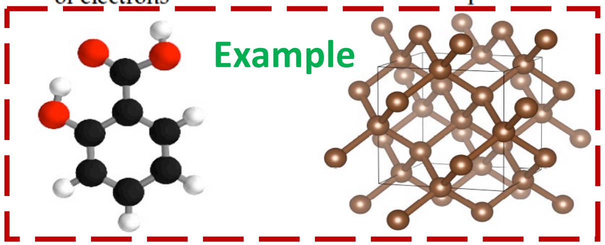




$$\hat{H} = \underbrace{-\sum_i \frac{1}{2m_e}\nabla_i^2}_{\text{kinetic energy of electrons}} \underbrace{-\sum_k \frac{1}{2M_k}\nabla_k^2}_{\text{kinetic energy of nuclei}} \underbrace{-\sum_i\sum_k \frac{Z_k}{d_{ik}}}_{\text{electron-nuclear attraction}} + \underbrace{\sum_{i<j}\frac{1}{d_{ij}}}_{\text{electron-electron repulsion}} + \underbrace{\sum_{k<l}\frac{Z_k Z_l}{d_{kl}}}_{\text{nuclear-nuclear repulsion}}$$

The quantum-mechanical Hamiltonian operator of charged particles (electrons and nuclei) interact among each other

$$E_0 = \underbrace{\bar{T}[\rho_0(\mathbf{r})]}_{\text{kinetic energy of electrons}} + \underbrace{\bar{V}_{\text{ne}}[\rho_0(\mathbf{r})]}_{\text{nuclear-electron attraction}} + \underbrace{\bar{V}_{\text{ee}}[\rho_0(\mathbf{r})]}_{\text{electron-electron repulsion}}$$



(a) Molecule: Salicylic acid (b) Bulk crystal: Diamond

$$\bar{E}[\rho(\mathbf{r})] = \underbrace{\bar{T}_{\text{ni}}[\rho_0(\mathbf{r})]}_{\text{kinetic energy of non-interacting electrons}} + \underbrace{\bar{V}_{\text{ne}}[\rho_0(\mathbf{r})]}_{\text{nuclear-electron attraction}} + \underbrace{\bar{V}_{\text{ee}}[\rho_0(\mathbf{r})]}_{\text{classic electron repulsion}} + \underbrace{\Delta\bar{T}[\rho_0(\mathbf{r})]}_{\text{interaction correction of kinetic energy}} + \underbrace{\Delta\bar{V}_{\text{ee}}[\rho_0(\mathbf{r})]}_{\text{non-classical electron repulsion}},$$

Definition of the energy functional as a system of non-interacting electrons

Thank You

for your attention