

KPP Simulator Multi-Phase Upgrade Blueprint

Foundational Audit of the Existing Codebase

Architecture & Code Structure: The current KPP simulator is a Python application with a Flask backend and a browser-based frontend. The repository audit reveals a basic structure where simulation logic and web interface are intermingled, making it Windows-specific and monolithic. Key modules (e.g. physics calculations, data handling) are not cleanly separated. This tight coupling between the Flask routes and simulation routines suggests a need for clearer separation of concerns and improved modularity. There is little evidence of a multi-layer architecture (such as distinct layers for physics models, simulation engine, and presentation). As a result, extending or replacing components (for example, swapping out the fluid dynamics module for a CFD engine) would currently be difficult due to hard-coded interdependencies.

Physics Modeling Gaps: The existing physics implementation appears to use simplified formulas and neglects several real-world effects. For instance, buoyancy might be implemented as a constant upward force without accounting for dynamic pressure variation with depth, or without adjusting for fluid density changes. (Buoyant force should follow Archimedes' principle – equal to the weight of displaced fluid ¹ – but any oversimplification here could reduce accuracy.) Drag forces on moving floaters may be modeled with a rudimentary linear damping or not at all; a proper drag force is proportional to velocity squared and depends on shape and fluid properties ², but the code does not show robust handling of hydrodynamic drag or lift. Thermal effects and gas behavior are likely omitted (e.g. assuming isothermal processes or ignoring heat exchange in compression). Electromagnetic aspects (like generator load) seem to be treated abstractly or with placeholders – for example, using a fixed efficiency factor rather than a dynamic electromechanical model. The power conversion from mechanical to electrical is probably simplified (perhaps using a constant torque or efficiency), rather than simulating the generator's electromagnetic response or back-emf under load.

Real-Time & Interactive Limitations: The current simulator runs on a single-threaded Flask server, which means the physics simulation is likely executed in the request context or via JavaScript in the browser. This setup can block the UI and cannot truly run *in real-time* while simultaneously updating the frontend. There is no evidence of a scheduler or simulation loop running asynchronously to achieve continuous time updates. The “real-time” experience is limited – users might have to start/stop simulation steps manually or endure noticeable latency between adjusting a parameter and seeing results. Moreover, no multi-floater capability exists yet: the simulation likely handles one floater (or one set of identical floaters) in isolation. Any attempt to simulate multiple floaters (e.g. several buoyant objects interacting or cycling through a tank) would require manually duplicating code or is simply not supported.

Data Management & Logging: The codebase does not implement robust data logging or time-series data management. Outputs are probably calculated on the fly and displayed, but not systematically recorded. There may be basic printing of results or simple charts, but no centralized logging utility or data export feature. This means users cannot easily retrieve simulation histories or perform post-run analysis, which is essential for a *professional-grade* simulator. In-memory data handling is ad-hoc – possibly using global

variables or simple Python lists to accumulate results, which will not scale well for long simulations or high-frequency time steps.

Software Quality: Documentation and testing appear minimal. Inline comments and docstrings are sparse, making it hard for new developers to grasp the code's intent. No formal test suite is present, indicating that verification of physics correctness relies solely on manual observation. Error handling is basic – for example, the simulator might not gracefully handle physically impossible inputs (like negative masses or extreme values) or numerical instabilities (e.g. it may crash or produce NaNs without clear messaging). The Windows-only limitation suggests the code might be using OS-specific calls (perhaps for serial port data or specific GUI elements) or simply hasn't been tested on Linux/Mac. There is a clear gap in cross-platform support, continuous integration, and use of best practices (like PEP8 style compliance, linting, etc.).

Summary of Gaps: In short, the existing KPP simulator provides a *proof-of-concept* but falls short of professional standards in accuracy, modularity, and interactivity. It lacks advanced physics modules (nanobubble effects, detailed thermodynamics, proper multi-body dynamics), a scalable architecture for extension, real-time performance, and integration of AI/CFD tools. These deficiencies set the stage for a comprehensive, phased upgrade plan to transform the simulator into a high-fidelity, extensible platform.

Multi-Stage Upgrade Roadmap

To evolve the KPP simulator systematically, we propose a multi-stage roadmap. Each stage focuses on incremental goals – improving physics fidelity, adding capabilities, and restructuring the architecture – while ensuring a working product at each milestone. Below is the structured plan with main stages and sub-stages:

- **Stage 1: Core Physics Refinement** – Enhance the fundamental physics models to achieve >95% real-world accuracy. This includes revamping buoyancy, drag, thermodynamics, and basic electromechanical conversion. Sub-stages:
 - *Stage 1A – Hydrodynamics & Buoyancy:* Implement accurate buoyant force calculations and fluid resistance. Use Archimedes' principle for buoyancy (force = weight of displaced fluid) ¹ and a drag force model $F_d = \frac{1}{2} C_d \rho A v^2$ opposing motion ². Calibrate coefficients (drag coefficient C_d , added mass, etc.) against known data to ensure the simulation responds realistically (e.g., terminal velocity of a floater in water matches expectation).
 - *Stage 1B – Thermodynamics & Compressibility:* Introduce proper gas law behavior for the air injection system. Model the air compressor and bubbles with thermodynamic processes – e.g. assume near-isothermal compression (heat dissipated to water) and apply ideal gas law $PV = nRT$ for pressure-volume changes. Include **isothermal absorption (H2)** of air in water: apply Henry's Law for gas dissolution at equilibrium (gas dissolved \propto partial pressure at constant temperature ³) to account for loss of air due to absorption (this affects bubble sizes and buoyancy over time).
 - *Stage 1C – Electromechanical Coupling:* Improve the representation of the generator and power conversion. Instead of a fixed efficiency, simulate the **mechanical-to-electrical conversion** by introducing a generator model where electrical load creates a counter-torque. For example, relate torque τ and angular velocity ω to electrical power P by $P = \tau \cdot \omega$ ⁴, and include an efficiency factor or dynamic model (perhaps a DC motor/generator equation with back-EMF). This means as more current is drawn (higher electrical load), the resistance (torque) increases, slowing the rotation – just as in a real KPP generator control system. Incorporate basic electromagnetism principles (e.g., generator coil inductance or magnetic saturation as needed for realism).

- *Stage 1D – Validation & Logging:* By end of Stage 1, establish a validation suite and logging. Compare simulation output with known benchmarks (e.g., a single floater’s rise time in water, or power output for a given float size) to ensure the >95% accuracy goal is on track. Implement a logging module to record time-series data of key variables (position, velocity, forces, pressure, torque, power, etc.) at each time step for analysis and debugging.
- **Stage 2: Real-Time Engine & Multi-Floater Simulation** – Transform the simulator into a real-time interactive application and allow simulation of multiple floaters (or multiple devices) concurrently.
 - *Stage 2A – Real-Time Simulation Loop:* Refactor the simulation to run as a continuous loop or background thread, decoupled from the web request/response cycle. Utilize a scheduler with a fixed time step (e.g., 0.01 s) to update physics in real-time. Ensure this loop can keep pace with wall-clock time for a reasonable system size, optimizing calculations via NumPy (vectorizing operations) or using C extensions for heavy computations. The frontend will connect via WebSocket or similar to receive periodic updates without blocking ⁵ ⁶. The target is an immediate GUI response as the simulation runs, aligning with modern simulation software expectations of *real-time computing and rendering* ⁷.
 - *Stage 2B – Multi-Floater Dynamics:* Expand the physics engine to support multiple floaters and their interactions. Architect the simulation core to handle an array of floater objects, each with its own state (position, velocity, etc.), but possibly coupled through shared resources like water and the connected mechanical system (e.g., if floaters are attached to a chain/belt driving a generator, their motion is linked). Implement collision handling or minimum spacing if floaters shouldn’t overlap. This stage will likely involve creating a **Floater class** to encapsulate individual floater properties and a higher-level **Simulation controller** to integrate them. The result will be a *multi-body simulation* where, for example, one floater entering the water while another exits can be visualized simultaneously.
 - *Stage 2C – Visualization & UI Improvements:* Upgrade the visualization to handle real-time updates from multiple moving objects. This could involve an animated 2D schematic (showing a side view of the water tank with floaters rising and falling) or even a 3D view for a more immersive depiction. Use a JavaScript library (e.g., D3.js or three.js) or a Python plotting library supporting live updates (Plotly Dash, Bokeh, etc.) to render motion smoothly. The UI will also gain controls to start/pause the simulation, adjust speed, and add or remove floaters on the fly. At this stage, the user can tweak parameters (like number of floaters, air injection rate, load resistance) and see the effects immediately in the running simulation.
- **Stage 3: Advanced Module Integration (H1, H2, H3)** – Incorporate specialized physical phenomena via modular expansions:
 - *Stage 3A – Nanobubble Interaction (H1):*** Introduce a module to simulate nanobubble effects in the water. Nanobubbles (ultrafine bubbles <1µm) can drastically alter fluid behavior – for instance, they can form a low-viscosity layer on surfaces, reducing drag ⁸. In the KPP context, if nanobubbles are generated (e.g., by electrolysis or special nozzles), they might reduce the friction on floater surfaces or enhance buoyancy. Implement this by adjusting the drag coefficient dynamically when nanobubbles are present, or by adding a “slip” effect in water (reducing effective water density or viscosity locally). The module should allow toggling nanobubble effects on/off and specifying parameters (bubble size distribution, concentration). Internally, this might hook into the drag force

calculation – e.g., if H1 is enabled, use a lower effective viscosity or boundary layer thickness to simulate drag reduction.

- **Stage 3B – Isothermal Absorption (H2):**** Extend the thermodynamics model to account for continuous absorption of air into water under isothermal conditions. This goes beyond Stage 1's static Henry's Law equilibrium by simulating the rate of absorption. Implement mass-transfer equations for gas absorption: when air bubbles are injected, a portion of the air dissolves into the water over time (at a rate depending on surface area of bubbles, saturation level of water, etc.). This will gradually reduce bubble volume (and thus buoyant force) as bubbles rise. Keep the process isothermal (constant temperature) to simplify – meaning the absorption does not significantly change temperature, and Henry's law constant remains applicable. This H2 module will introduce time-dependent bubble size or mass of dissolved gas in the water. It ensures the simulator reflects phenomena like diminishing buoyancy for long-rising bubbles or the need for water de-gassing systems in real KPP operations.
- **Stage 3C – Air-Injection-Induced Torque (H3):**** Develop a module to capture how the act of air injection itself can impart torque or disturb the system. In real KPPs, when compressed air is injected into a floater at depth, there could be a reactive force (Newton's third law: the water and float experience a kick from the air jet) that might contribute to turning the chain or oscillating the floater. To simulate this, model the injection as a short impulse force or torque at the moment of bubble release. For example, when a floater at the bottom gets injected with air, apply an upward force (already in buoyancy) but also a slight rotational impulse to the chain mechanism (because the air rush might push on a turbine or the floater in a certain direction). This H3 module will likely interface with the mechanical dynamics: e.g., increasing the effective torque on the main shaft during injection events, or adding a momentary acceleration to the floater. Parameters will include injection pressure, nozzle direction, etc., to tune the magnitude of this effect.
- **Stage 3D – Modular Integration & Testing:** Each of the above modules (H1, H2, H3) is developed as a **pluggable component**. The architecture should allow these modules to be enabled or disabled via configuration. That means clear interfaces: e.g., the core simulation calls `H1.update_drag(floater)` if H1 is active, or `H2.absorb(bubble)` each time step if H2 is active, etc. We will document and test each module in isolation (unit tests using controlled scenarios: e.g., in a still water tank, does the H2 model eventually equalize dissolved gas to Henry's law value? Does H1 reduce drag force as expected?). This modular approach aligns with weakly coupled multi-physics design, making it easier to maintain and extend ⁹.
- **Stage 4: Scalable Architecture and OpenFOAM Compatibility** – Re-engineer parts of the simulator to be enterprise-grade and prepare for future high-fidelity CFD integration.
- **Stage 4A – Architecture Refactoring:** Evolve the codebase into a **layered architecture**. Separate the code into distinct layers or packages: for example, `physics_core` (all physics calculations and models), `simulation_engine` (time-stepping logic, scenario setup, managing multiple solvers), `data` (data schemas, logging, import/export), and `web_interface` (Flask app or web server code). Within `physics_core`, further organize by domains (fluid dynamics, thermodynamics, mechanical, electrical). Define clear APIs between components. For instance, a `Floater` class (in fluid module) might provide a method to compute net forces given environmental inputs, and the mechanical module's `RotationalSystem` class might use that to update angular velocity. This refactor ensures the simulator is modular at the code level: developers can swap out the fluid solver (e.g., replace our internal calculations with OpenFOAM calls) without touching the UI or other parts.

Emphasize *in-memory processing* – data should be passed through memory (or via fast inter-process communication) rather than written to disk frequently, to keep simulation speeds high.

- **Stage 4B – Performance Optimization:** As the simulator grows in complexity, ensure it remains performant. Profile the code to identify bottlenecks. Introduce parallelism or vectorization where possible – for example, use NumPy for array calculations of forces on many floaters simultaneously, or use Python's `multiprocessing` or asynchronous programming to offload tasks (like each module H1/H2 running concurrently on separate cores). Consider employing **Numba** (Just-In-Time compilation) or writing critical loops in Cython/C++ for speed. The goal is to allow larger simulations (e.g., tens of floaters, long durations) to run faster than real time, if possible, so that what would be 1 hour of real operation can simulate in minutes on a desktop. This stage might also include making the code cross-platform (removing any Windows-specific calls, using cross-platform libraries) so it can run on Linux servers or be containerized for deployment.
- **Stage 4C – OpenFOAM Preparation:** Begin integrating with CFD for fluid dynamics. OpenFOAM is a powerful open-source CFD tool; to leverage it, we plan the following:
 - **Data Exchange Formats:** Ensure our simulation can export geometry and flow conditions in a format OpenFOAM understands (e.g., generating a mesh or parameter file). Define an interface where, for example, the shape and path of floaters can be sent to an OpenFOAM case directory for a finer analysis.
 - **Loose Coupling Mode:** At first, implement an *offline coupling* – e.g., run our simulation with a simplified fluid model, but at certain intervals or for certain scenarios, output a snapshot (floater positions, velocities) and invoke OpenFOAM (via a Python wrapper or system call) to compute detailed pressure/flow fields. The results can then inform adjustments to our model (like refining drag coefficients). This can validate and improve our simpler models without running full CFD every step.
 - **Future Tight Coupling:** Design the architecture such that replacing the internal fluid solver with OpenFOAM in real-time is feasible. For example, encapsulate fluid force calculations behind an interface `FluidSolver.compute_forces(objects, state)`. We can implement two versions of this: a fast analytical model (used normally) and an OpenFOAM-backed model (which might run slower). In final deployment, a user could choose CFD mode for highest accuracy, at the cost of speed. We will investigate using libraries or APIs (like PyFOAM or a custom OpenFOAM plugin) to call OpenFOAM solvers from Python, possibly in parallel to maintain interactivity. Stage 4C ensures that by the end of Stage 4, the simulator is *CFD-ready*: all necessary hooks and data structures are in place for full CFD integration in Stage 5.
- **Stage 5: AI-Augmented Simulation & Design Module** – Final stage adds artificial intelligence tools to assist users in optimizing and tuning the KPP design.
- **Stage 5A – AI Design Advisor:** Develop an AI module that can analyze simulation outputs and suggest improvements. This could leverage machine learning on simulation data or rules derived from domain expertise. For example, implement a reinforcement learning or optimization algorithm that adjusts certain parameters (float size, injection timing, ballast weight, etc.) to maximize output power or efficiency. The AI module would run multiple simulation iterations (possibly in a batch or accelerated mode) to search for optimal configurations. Results can be presented to the user as recommendations ("e.g., **Suggestion:** Increase float volume by 10% to improve generation by 5%").

Because our software is modular, this AI can interface via the same APIs the UI uses – essentially programmatically tweaking inputs and reading outputs.

- *Stage 5B – Predictive Maintenance & Anomaly Detection:* Leverage AI in another way: use it to monitor the simulation (or real data if connected to a live system) for anomalies or inefficiencies. By training models on normal simulation runs, the system can flag when a certain variable deviates beyond expected bounds (e.g., if a floater’s rise time is slower than predicted under current settings, indicating possible issues like increased drag or leakage). This adds a layer of intelligence to the simulator, making it not just a passive tool but an active advisor for system health and performance.
- *Stage 5C – User-Facing AI Tools:* Integrate simpler AI features into the UI for user convenience. For example, an **auto-tune** button that runs a quick optimization on one parameter (like finding the ideal air injection rate for current conditions) or an AI chat assistant that can answer “what-if” questions (backed by the simulation and a knowledge base from prior runs). While these are auxiliary, they position the KPP simulator as a cutting-edge platform that uses data-driven insights, aligning with modern trends where “data exchanging interfaces for AI-based automation” are expected ¹⁰.
- *Stage 5D – Final Testing & Deployment:* At the end of this stage, conduct comprehensive testing of the entire platform. This includes physics validation (all new features produce physically sensible results), performance testing (real-time goals met; the system handles expected loads), and user acceptance testing (the UI and AI features are intuitive and helpful). Documentation is finalized for all modules. The result is a professional-grade KPP simulation platform that is *CFD-enhanced* for accuracy and *AI-augmented* for user guidance, ready for deployment on Windows and other environments (with potential cloud or HPC deployment in the future).

Each stage above builds on the previous, ensuring that at no point is the simulator in an unusable state. Stakeholders could potentially use the simulator at the end of each stage (Stage 1 for improved accuracy single-floater studies, Stage 2 for real-time demos, Stage 3 for specialized physics experiments, etc.), while we continue to enhance it in subsequent stages.

Detailed Architectural Blueprint

A robust architecture is critical for a high-performance simulator. We propose a modular, extensible software design that separates concerns and allows easy integration of new features like CFD solvers or AI components. Below is the target architecture and project structure:

Project Structure: Organize the repository into clear directories/packages:

- `kpp_simulator/` – Main Python package for the simulator.
- `physics/` – All physics models and calculations.
 - `fluid_dynamics.py` – Functions/classes for buoyancy, drag, pressure calculation. (E.g., a `FluidSolver` class with methods to compute forces on floaters, given fluid properties.)
 - `thermodynamics.py` – Gas laws, heat transfer, absorption calculations. (Could define a `GasBubble` class tracking bubble radius, or functions for isothermal absorption rates.)
 - `mechanics.py` – Rigid body mechanics and kinematics. (Includes gravity force, equations of motion integrators, perhaps a `Floater` class combining fluid forces + mechanical state.)
 - `electrical.py` – Generator and electrical load model. (E.g., a `Generator` class that given shaft speed and field parameters computes electrical output and counter-torque.)

- `special/` – Sub-package for special modules (H1, H2, H3). Each of H1, H2, H3 can be a sub-module or class:
- `nanobubble_effects.py` – containing functions to modify drag or other properties when enabled.
- `absorption.py` – functions for Henry's law and absorption kinetics.
- `injection_torque.py` – functions to calculate impulse forces/torques from air injection.
- `simulation/` – Core simulation engine.
 - `sim_engine.py` – Manages the time loop, updates all entities per time step, and orchestrates interactions. For example, this engine will call out to physics modules: compute forces, advance positions, update generator state, etc., each tick.
 - `entities.py` – Definitions of main entities like `Floater`, `Tank`, `PowerTrain`. A `Floater` object contains properties (mass, volume, position, velocity, etc.) and maybe methods like `apply_forces()` which use physics.physics modules. `Tank` might hold global properties (water depth, fluid density, maybe list of bubbles if tracking individually). `PowerTrain` might represent the mechanical connection from floaters to generator (e.g., a belt or gear ratio).
 - `solver.py` – Could contain numerical solvers (integrators). For instance, an implementation of Runge-Kutta or simpler Euler integrator to update ODEs each time step. Using a stable integration method is important for accuracy in the dynamic simulation.
 - `scenario.py` – Handles set-up of different simulation scenarios or configurations (e.g., number of floaters, their initial positions, etc.), possibly reading from a config or UI inputs.
- `data/` – Data management.
 - `logging.py` – Utilities for logging simulation data to memory structures or files. Could define a `DataLogger` that collects time-series in Python lists or NumPy arrays and writes to CSV/JSON or even a lightweight database if needed.
 - `analysis.py` – Basic analysis or calculation routines (e.g., summarizing efficiency, computing totals) that can be used by the AI module or for post-processing results.
 - `io/` (if needed) – for any file I/O, like exporting to OpenFOAM case files or reading configuration. For OpenFOAM, e.g., an `openfoam_writer.py` to output current state in OpenFOAM formats.
- `ai/` – AI and optimization tools.
 - `optimizer.py` – Functions or classes for running optimization loops on simulation parameters (could implement a simple genetic algorithm or connect to a library like SciPy's `optimize` or an RL library).
 - `anomaly_detection.py` – If using any ML models for anomaly detection, those classes or model loading code would go here.
 - (This module might expand with sub-packages if using complex AI frameworks or pre-trained models.)
- `webapp/` – The Flask web application and any front-end assets.
 - `app.py` – Flask application initialization, routes.
 - `routes.py` – Define API endpoints (e.g., start simulation, get latest data, adjust parameter endpoints).
 - `sockets.py` – Setup for WebSocket communications (using Flask-SocketIO or similar) to stream simulation updates to the client in real-time.
 - `static/` – Static files (HTML, CSS, JS for the front-end). Possibly include a JavaScript UI built with a modern framework (or simple vanilla JS) to render visualization and controls.
 - `templates/` – HTML templates if using server-side rendering for any pages.

- `tests/` - Test suite.
 - `test_physics.py`, `test_simulation.py`, etc. to verify that each component works as expected.

Modularity and Interfaces: Each module above has a well-defined interface: - Physics modules should contain pure functions or classes that *do not depend on the rest of the system*. For example, one can call a buoyancy function with given volume and fluid density to get a force, without any global state. This makes them easily testable and replaceable. The `Floater` class can use these functions internally, but the functions themselves stand alone (and could be swapped out for, say, a more complex CFD call). - The simulation engine (`sim_engine.py`) interacts with floaters and other entities through abstract interfaces. For instance, it might call `floater.compute_net_force()` each step, which internally sums gravity, buoyancy, drag, etc. If later we integrate OpenFOAM, we could override `compute_net_force` to get forces from a CFD computation instead of our analytical model. - Communication between modules uses data structures like Python dictionaries or dataclasses to package state information. For instance, after each time step, the simulation engine could produce a dictionary of results (`{'time': t, 'floaters': [...], 'generator': {...}}`) that is handed off to the logging system and the WebSocket broadcaster. This decoupling means the logger and UI don't need to know internal details of the simulation objects - they just consume structured data.

Calculation Pipeline: The main loop each simulation tick might look like: 1. **Input Gathering:** Read any control changes (e.g., user adjusted a valve or load via UI) and update simulation state accordingly. 2. **Physics Update:** For each floater (and other moving parts): - Calculate forces: buoyancy from fluid (via `fluid_dynamics`), drag from fluid (via `fluid_dynamics`), weight (via `mechanics`), etc. Also, if H1/H2/H3 are active, apply their contributions: e.g., adjust drag for H1, reduce buoyant force for H2 if bubble shrank, add injection force for H3 if at injection event. - Sum forces to get net force, then integrate acceleration to update velocity and position (using `solver.py` integrators). - For rotation (if modeling a chain or wheel), compute net torque from all floaters on the shaft plus generator resistive torque from `electrical` module. Update angular speed accordingly. - Update the state of the generator/electrical system: given new angular speed, compute new electrical power output (and possibly feed this into a simple circuit model if needed for realism). - Handle interactions: if one floater reaches top of tank, maybe it exits water and another enters at bottom (for a continuous chain, you'd teleport or cycle the object's position). This requires carefully managing the list of floaters (could treat them in a circular buffer fashion). 3. **Data Logging:** Collect key state variables (positions, velocities, pressures, power, etc.) and pass to the logger. 4. **Real-Time Broadcast:** Send updated state to the UI via WebSocket (perhaps at a lower frequency than the physics tick - e.g., physics at 100 Hz, but send to UI at 20 Hz to reduce overhead). 5. **Loop Timing:** Ensure the loop waits or adapts to maintain real-time pace (e.g., using `time.sleep` for fixed step or adjusting step size dynamically if running behind).

This pipeline is designed for in-memory speed. All computations happen within Python's memory space (with optimized math libraries) and only small JSON messages go out to the UI. There's no disk I/O in the loop except optional periodic logging flushes to file (which could be done asynchronously to avoid slowing the simulation).

Libraries & Tools: We will leverage proven libraries throughout: - **NumPy/SciPy:** for efficient numerical computations (matrix operations, ODE solvers if needed, interpolation, etc.). - **PyDy or SymPy (optional):** for deriving equations of motion if we formulate some of the mechanics symbolically. - **Flask-SocketIO or websockets:** for real-time bi-directional communication between backend and frontend. - **Plotly/Bokeh/**

Three.js: for visualization. For example, use Plotly for plotting time-series graphs (power output vs time) and Three.js for a 3D model of the KPP (if a 3D view is desired in browser). These libraries can be integrated such that the Python backend sends data and the JS library in frontend renders it. - **OpenFOAM/PyFOAM:** for CFD integration. We won't rewrite OpenFOAM in Python; instead, we either call OpenFOAM externally (through system calls or using a Python wrapper to manipulate case files and run solvers). The architecture just needs to ensure we can export our simulation state to OpenFOAM and read results back. We might use the `PyFoam` library (which provides Python utilities to run OpenFOAM cases) or write a custom interface. - **AI libraries:** Depending on needs, we might use frameworks like scikit-learn for simple regression or clustering (for anomaly detection) and stable-baselines or TensorFlow/PyTorch if implementing reinforcement learning for optimization. These would reside in the `ai/` module and be used offline (not to slow down the main sim loop).

Extensibility: The design allows new modules to be added with minimal changes to existing code. For instance, if a new phenomenon H4 (say, water salinity effects on buoyancy) needs to be added, we can create `physics/special/salinity.py`, and then simply plug it into the simulation loop (adjust buoyancy calculation by a factor from H4). The rest of the system doesn't need overhaul. Similarly, if a new visualization tool or output format is needed, it can be added in the `webapp` or `data` layer without touching core physics.

Throughout development, we will maintain documentation of the architecture (UML diagrams of class structure, flowcharts of the simulation loop). This ensures every team member and new contributors can quickly understand how data flows through the system and where to make changes for specific improvements.

Mathematical Model Coverage

The upgraded simulator will cover a comprehensive range of physical models. Below we enumerate the key forces, dynamics, and equations that will be implemented or refined, ensuring no critical physics is omitted:

- **Buoyancy (Upthrust):** Modeled via Archimedes' Principle. Every submerged floater experiences an upward buoyant force equal to the weight of the displaced water ¹. Formula: $F_b = \rho_{\text{water}} V_{\text{disp}} g$, where V_{disp} is the submerged volume. The simulator will compute V_{disp} based on floater geometry and submersion depth (which may vary if the floater is not fully submerged). This accurately captures that deeper or larger floaters get more buoyant force until fully submerged. The buoyancy will automatically balance with gravity in steady-state (floating condition) or produce acceleration if unbalanced (rising or sinking motion).
- **Gravity & Weight:** Each floater has weight $F_g = m g$ acting downward. This is straightforward but crucial for dynamics (especially for partially submerged or when evaluating net force = buoyancy - weight - drag, etc.). We also account for gravity in other parts: the whole chain and generator load have weight (which might matter if orientation isn't purely vertical - though in KPP we assume vertical motion primarily).
- **Hydrodynamic Drag:** As floaters move through water, they encounter drag resistance opposing their motion. We use the quadratic drag law: $F_d = \frac{1}{2} C_d \rho_{\text{water}} A_{\text{proj}} v^2$ in the opposite direction of velocity ². Here C_d is the drag coefficient (depends on shape - e.g., a streamlined floater vs. a flat plate), A_{proj} is the projected area in the direction of motion, and v is relative velocity of the floater through water. We will incorporate both *form drag* (pressure drag) and potentially *viscous drag* if

needed (though for large objects like floaters, pressure drag dominates). In addition, if the floater oscillates or if there's water flow, Reynolds number regime will be considered – but since KPP typically has low-speed buoyant rise, flow is laminar around floaters. Still, we can allow the user to input a custom C_d , or even a table of $C_d(Re)$ to increase fidelity for different speeds.

- **Added Mass and Fluid Inertia:** When an object accelerates in a fluid, it effectively carries some surrounding fluid with it (added mass effect). For high accuracy, especially in transient motions, we can include an added mass term in the equations of motion. This means the effective inertia of a floater is $m + m_{\text{added}}$, where m_{added} depends on the shape and displaced fluid mass. This will slow down acceleration slightly, matching real observations.
- **Hydrostatic Pressure:** The simulator will consider water pressure increasing with depth: $P_{\text{water}}(h) = \rho_{\text{water}}gh + P_{\text{atm}}$. This is mainly used indirectly (for buoyancy calculation, since buoyancy can be derived from pressure differential with depth). If needed, we will compute the pressure at various points (e.g., at injection nozzle depth to know required compressor pressure to inject air).
- **Air Compression & Gas Laws:** Air injection is a core part of KPP. We will model the compressor and injection using thermodynamics:
 - Use the **Ideal Gas Law** for the air in floaters: $PV = nRT$. If injection is quick and water provides cooling, we approximate it as isothermal (T constant) so $P \propto \frac{n}{V}$. Before injection, the floater is filled with water; after injection, a certain volume of air at pressure is inside. We'll calculate how much air (moles or mass) is injected based on compressor pressure and depth (must exceed water pressure at that depth).
 - **Isothermal absorption (H2):** Henry's Law will govern dissolution: at equilibrium, concentration of air in water $C = k_H P_{\text{air}}$ (with k_H Henry's constant). We'll implement a first-order absorption rate: $\frac{dC}{dt} = k(C_{\text{equil}} - C_{\text{current}})$ for the water immediately around bubbles, ensuring the system gradually approaches equilibrium. This affects bubble size: as air leaves the bubble into water, bubble volume shrinks, reducing buoyant force. We also track total gas lost over time, which slightly reduces efficiency (in real systems, undissolved gas is recirculated).
 - **Thermal Effects:** While we assume isothermal for simplicity initially, we note that real compression is not perfectly isothermal. In advanced stages, we might let the user switch to an adiabatic model for compression (using $PV^\gamma = \text{const}$ for air, with $\gamma \approx 1.4$ for diatomic gas) and include heat exchange with water by a simplified model (e.g., a time constant for heat dissipation). For now, maintaining Stage 1's isothermal assumption suffices for ~95% accuracy since water bathes the floats and acts as a large heat sink.
- **Multiphase Fluid Consideration:** The presence of both water and air (bubbles) in the system technically makes it a multiphase flow. Our approach is to treat the floater plus its bubble as one system for forces, and handle the mass exchange via H2. We won't simulate water flow around bubbles at CFD level until OpenFOAM integration, but we ensure effects like buoyancy change due to bubbles are included. If needed, we incorporate a *buoyancy boost* for rising bubbles (the "airlift" effect) separate from floater buoyancy.
- **Torque and Rotational Dynamics:** A crucial aspect is the conversion of linear motion of floaters to rotational motion of the generator. In KPP, typically floats are attached to a belt or chain that turns a wheel (and generator). We will model the **rotational dynamics** of that system:
 - Define a moment of inertia I for the rotating assembly (wheel, generator rotor). The net torque on this system comes from floaters (upward force * lever arm) minus generator resistive torque and friction.

- As floaters rise on one side, they apply an upward force on the belt; on the other side (descending floats, if any), gravity might assist or oppose depending on design. We sum all these contributions to get net torque on the shaft.
- Use Newton's rotational equation: $I\alpha = \tau_{\text{net}}$ to update angular velocity (where α is angular acceleration).
- The **generator model** provides a braking torque $\tau_{\text{generator}}$ that depends on electrical load. For example, for a simple generator: $\tau_{\text{generator}} = kI_{\text{elec}}$ (current times a constant), and I_{elec} relates to voltage and load resistance. Rather than simulate electrical circuits in detail, we can use the known fact that $P_{\text{electrical}} = VI = \tau\omega$ ⁴. If the user specifies an electrical load (resistance or desired power draw), the code can compute the corresponding torque that would yield that power at the current speed. We'll also include generator efficiency (not all mechanical power converts to electricity, some lost as heat).
- **Friction and Damping:** Include mechanical friction in bearings or water (if any moving parts in water) as a constant small torque or linear damping on rotation. This prevents unphysical perpetual motion and captures real inefficiencies.
- **Floaters' Vertical Motion:** Modeled by Newton's second law in vertical direction for each floater: $m_{\text{floater}} \frac{dv}{dt} = F_b - F_g - F_d + F_{\text{inject}}$. Here F_{inject} represents any extra force from air injection (H3), applied impulsively or over a short time when air is injected. We integrate this ODE for velocity and position over time. Constraints: the floater cannot penetrate beyond the water surface (once it reaches top, it exits or hits a stopper) – we will handle that by resetting or clamping position and possibly transferring that floater to bottom if recycling in a loop.
- **Water Level and Tank Dynamics:** In a closed tank, adding air displaces water, possibly changing pressure or water level slightly. We assume the tank is vented (constant atmospheric pressure on top) and large enough that water level change is negligible. If needed for extreme accuracy, we can include water level change: as floats and bubbles rise, they might push water out (which could matter in a small tank). For now, this is minor and can be ignored or left static.
- **Electrical Dynamics:** If integrating with a grid or battery, the electrical side could be simulated (voltage, current). That might be beyond scope, so we keep it simple: either assume the generator is connected to an ideal load that takes whatever power is produced (so we just calculate power), or allow the user to specify a load and we compute how much power actually flows given the mechanical input.
- **Control Systems (future):** KPP might involve control (e.g., controlling compressor to maintain a certain RPM). We plan for potential PI controllers in the simulation if needed (for example, an automatic air injection timing control to regulate speed). Those would be simple algorithmic additions in the simulation loop, ensuring the simulated system can be operated in a controlled manner.

All mathematical models will be verified individually: - We will compare buoyancy calculations against known values (e.g., does a 1 m³ floater in water get ~9800 N of upthrust?). - Drag models can be verified using known drag coefficients (for a sphere, etc.) and checking terminal velocity calculations. - Thermodynamic changes (isothermal vs adiabatic compression) can be checked with textbook examples (compression of air from 1 atm to 3 atm, etc.). - The torque/power calculations will be cross-checked: e.g., if one floater provides X N force over a 1 m lever arm, that's X Nm torque; at a certain RPM, does the power match $\tau\omega$. - This thorough coverage of forces and equations ensures the simulator can mimic real-world physics to >95% accuracy as required. By Stage 4 or 5, any remaining discrepancies can be ironed out by the CFD integration (for fluid forces) or by fine-tuning parameters to match experimental data.

Logging, Visualization, and User Interface Goals

Each development stage includes clear targets for data logging, visualization quality, and user interface (UI) enhancements. By the final product, the simulator will not only be scientifically accurate but also user-friendly and visually insightful.

Logging and Data Management: From Stage 1 onward, the simulator will incorporate robust logging of simulation data: - Implement a **time-series logging system** that records all relevant variables at each simulation timestep (or at a user-specified sampling rate). This includes positions, velocities, accelerations of floaters; pressure and temperature values; generator speed and power output; etc. The logger will store data in memory during the run (using Python structures or pandas DataFrames) and have the ability to save to disk (CSV or HDF5 format) when the user requests or when the simulation ends. - Ensure that logging has minimal performance impact by allowing the user to choose logging frequency (log every step for detailed analysis, or every Nth step for long runs). We may use a ring buffer for data if memory is a concern for very long simulations, or stream data to disk incrementally in a separate thread. - Provide an **export feature** in the UI to download logged data for offline analysis (e.g., a CSV file of time-series). This is important for a professional tool, enabling engineers to use external tools (Excel, MATLAB) if needed on the simulation results. - The log module will also automatically compute summary statistics: e.g., total energy generated, peak forces, etc., and could produce a short report at the end of a run.

Real-Time Visualization: Visualization is pivotal for understanding simulation behavior. We will implement dynamic visualization that evolves through the stages: - **Stage 1/2 Visualization:** Start with 2D plots and basic animation. For example, a side-view diagram of the tank: water represented as a rectangle, and a circle or rectangle representing the floater moving up and down. This can be done with simple HTML5 canvas drawing or using a high-level library (like Plotly's animated scatter plot, or Matplotlib updating in the browser via Flask endpoints). Additionally, plot graphs in real-time: e.g., a strip-chart of generator power vs. time, or floater velocity vs. time. These give quantitative feedback alongside the qualitative animation. - **Multi-Floater View:** When multiple floaters are in play (Stage 2B), the visualization will show all floaters. Possibly depict a cutaway of the cylindrical tank with multiple floaters spaced around the circumference for clarity. If the KPP is conceptualized as a chain of buckets, we can draw multiple objects attached to a moving belt. - **Improving Realism:** By Stage 3+, move to more polished visuals. Incorporate 3D if beneficial: for instance, render floaters as 3D objects (cylinders or spheres) in a WebGL context (three.js) so the user can rotate and inspect. Show water surface and perhaps bubbles rising (as small particles) if H1/H2 are active. Real-time visualization should also highlight the effects of modules: e.g., when H1 nanobubbles are on, perhaps color-code the floater or water to indicate reduced drag regions. - **Performance Consideration:** Use efficient drawing methods for real-time. WebSocket will transmit state, and the client (browser) will handle rendering at e.g. 20 frames per second. We'll ensure to send only necessary data to avoid overload (for example, sending the coordinates of floaters and key numbers, rather than full field data). The visualization updating should be smooth for a good user experience.

User Interface and Controls: The front-end will evolve into a control panel for a virtual power plant: - Provide interactive controls for all adjustable parameters: sliders, dropdowns, or input boxes for things like: number of floaters, floater size/volume, floater mass, water density (to simulate fresh vs saltwater), compressor pressure, injection interval, generator load (resistance or target power), and toggles for the H1/H2/H3 modules. - Include *pre-set scenarios* the user can load (via a dropdown or menu). For example, "Single Floater Test", "Full 5-floater KPP", "High Load Scenario", etc., which automatically set multiple parameters to demonstrate certain behaviors. - **Real-Time Control:** For critical controls (like air injection rate, or load),

implement them in a way that user changes immediately affect the running sim. This may involve sending a command to the backend to update a parameter and the simulation loop reading it (as mentioned in the simulation pipeline). For example, the user could drag a slider to change generator load while the sim is running and see the floaters slow down in response – mimicking how an operator might control a real plant. - Display numeric readouts and gauges: e.g., current electrical output (kW) in big text or gauge, current RPM of generator, perhaps efficiency (%) and other performance metrics updated live. This gives a dashboard feel, useful for engineering analysis. - **Logging & Analysis UI:** After or during a run, allow the user to inspect logged data in the interface. This could be simple, like clicking a “Show Plots” button to generate a matplotlib or Plotly plot of certain logged quantities (e.g., power over time, or buoyant force over depth). For final stages, we might incorporate a small analysis toolbox where the user can choose variables to plot against each other. - **Error and Status Messages:** The UI should clearly display status (Running, Paused, Completed) and any warnings (e.g., “Warning: Floater 3 reached top and was reset” or “Nanobubble module active: drag reduced by 20%”). If the simulation detects any issues (like numerical instability or extreme conditions), show an alert to the user (and also handle it in code to avoid crashes). - **Responsiveness and Theme:** Make the UI professional and clean. A modern web design (using a library like Bootstrap or Material design for consistent styling) will be applied. Ensure the layout is responsive so it can be viewed on different screen sizes if needed (though as a desktop app primarily, we optimize for at least laptop screens). - Possibly include a help section or tooltips on UI controls explaining each parameter (since this is for a high-performance engineering team, but still helpful for new users).

By final deployment, the user interface will function as a **control room dashboard** for the KPP simulator: they can configure the plant, run the simulation in real-time, observe it much like an operator would observe gauges and the physical machine, and glean insights from both visuals and data. This level of interactivity and clarity is crucial for a professional-grade tool.

Final Stage: CFD Integration and AI Modules

In the concluding stages of the upgrade, we integrate the CFD and AI components to meet the project’s ultimate goals: a simulator that can leverage high-fidelity physics (through OpenFOAM) and provide intelligent assistance in design and optimization.

CFD Plug-In Support (OpenFOAM Integration): By Stage 4C, we set the foundation, and now we fully realize CFD integration: - **Embedded OpenFOAM Simulations:** We will allow the user to toggle a “CFD mode” for the fluid dynamics. In this mode, whenever fine fluid detail is necessary (for example, computing the precise drag or flow patterns around floaters), the simulator will launch an OpenFOAM case in the background. We’ll create simplified 2D or 3D CFD cases representing our scenario (e.g., a 2D axisymmetric column of water with a moving floater, or a 3D if needed). OpenFOAM can compute pressure, drag, lift with much higher accuracy than our analytical model. The results (drag force, pressure distribution) are fed back into the simulator. - **Co-simulation Approach:** Given that running a full CFD every time step is computationally expensive, we adopt co-simulation strategies. For instance, run the main simulation with an analytical model but periodically synchronize with CFD: - Do a brief CFD run at key moments (maybe at steady-state velocity of a floater, or when a new module effect is introduced) to calibrate our model parameters. E.g., OpenFOAM might tell us the drag coefficient more accurately for the current Reynolds number, and we then update our C_d in the fast model. - Alternatively, run a parallel thread where OpenFOAM continuously simulates one cycle of a floater’s motion in more detail, and use those results to correct the real-time sim (a form of real-time model correction). - **Data Exchange:** The simulator will generate necessary inputs for CFD: geometry of floater (which could be a simple shape in OpenFOAM’s

mesh), initial conditions (floater velocity, etc.). We'll script this using Python – possibly writing a `.csv` or directly editing OpenFOAM dictionaries. After OpenFOAM solves, we parse the outputs (drag force, etc.) either from logs or by sampling fields. The tight integration might use a tool like **swak4Foam** or the OpenFOAM Python bindings if available, to control simulation steps and get results. - **Use Cases for CFD Mode:** A user might activate CFD mode when they want to study detailed fluid behavior – for instance, to see flow separation, vortex formation, or to evaluate nanobubble effect at micro-scale. In our UI, we can offer a “CFD Analysis” button which, when clicked, pauses the real-time sim, runs an OpenFOAM simulation for the current state (maybe just one floater's scenario), and then displays the CFD results (we can visualize the flow field or at least give refined force values). This is invaluable for validation and for convincing stakeholders of accuracy, as CFD is often considered a benchmark. - **Ensuring Compatibility:** We make sure that our licensing and environment support OpenFOAM (which is open-source) and that the user has it installed if needed. Our code will detect if OpenFOAM is available; if not, CFD mode is disabled gracefully. We maintain general compatibility, so if later someone wants to plug in a different CFD solver, the interface in our code (FluidSolver interface) can accommodate that as well, not tying strictly to OpenFOAM specifics.

AI-Assisted Design and Tuning: The AI modules introduced in Stage 5A and 5B will be fully integrated and user-accessible: - **Design Optimization Workflows:** Provide templates for common optimization goals. For example, “Maximize Output Power” or “Minimize Compressor Energy for Given Output”. When the user selects such a goal, the simulator's AI module will vary design parameters through multiple simulation runs. This could use algorithms like Genetic Algorithms or Particle Swarm Optimization under the hood. Because brute-force can be slow, we might limit the number of parameters or use surrogate modeling (train a simple ML model on a few simulations to predict outcome, then optimize that model). The result is presented as recommended parameter sets. This helps engineers explore the design space efficiently. - **Machine Learning Integration:** We may train neural networks as surrogate models for the simulation. For instance, a neural net could learn the relationship between a set of input parameters (number of floaters, float volume, injection rate, load) and outcomes (power output, efficiency). Once trained (on simulation data), such a model can instantly predict outcomes, enabling near real-time optimization suggestions without running full physics each time. This is especially useful when linking with external optimization or when the user drags a slider – an AI prediction can give immediate feedback on expected outcome before the simulation catches up. - **AI for Anomaly Detection:** If this simulator is later connected to real KPP hardware, an AI could compare live data to simulation predictions to flag anomalies. Within the sim, we mimic that by having the AI watch for unusual patterns. For example, if enabling nanobubbles should reduce drag, but the simulation shows increased drag, the AI can pop-up a message: “Check nanobubble parameters – observed drag doesn't match expected reduction,” indicating either a bug or a situation outside training data. This kind of feature requires machine learning models to be trained on normal conditions and then detect outliers. - **User Interaction with AI:** The UI might include an “AI Assistant” panel. Users can ask natural language questions (“How can I increase efficiency?”) – the assistant would parse that and either run an optimization or retrieve information from simulation knowledge base to answer. While full NLP may be ambitious, we can at least provide guided Q&A like FAQs with dynamic content (e.g., after a run, user clicks “AI Insight: Why did power drop at 50s?” and the AI identifies that “the generator load was increased at 50s causing RPM to drop and power to stabilize at a new lower point” – essentially an explanation based on logged data). - **Continuous Learning:** Build the framework such that the AI models improve over time. As users run more simulations (or feed real data), we accumulate a dataset. We could allow an optional cloud-connect or central database (if this tool is used by a team) where simulation results are stored. The AI module can then retrain periodically on more data, improving its recommendations. This goes beyond initial scope, but our modular design means the AI can be updated independently of the physics engine.

In implementing the above, we adhere to **best practices for AI integration**: the AI suggestions are advisory and explainable (we'll provide context like "Based on 100 simulations, the best configuration had X, Y, Z"). The user always remains in control – AI won't change parameters unless the user applies a suggestion.

By completing CFD and AI integration, the KPP simulator transcends being just a calculator – it becomes a *comprehensive simulation platform*. Engineers can trust its physics (validated by CFD) and leverage its AI guidance to innovate faster. This combination is cutting-edge and positions the simulator as a potential industry-standard tool for kinetic power plant design.

Best Practices and Development Guidelines

To ensure the simulator remains reliable, maintainable, and extensible, we will follow software engineering best practices throughout the development:

- **Modularity and Encapsulation:** All code will be written with a modular mindset ⁹. Each class or function has a single responsibility, and different concerns (UI vs physics vs data management) live in different modules. This makes the codebase easier to navigate and reduces the risk of unintended side-effects when modifying a component. For example, changes in the visualization code won't break the physics engine, and vice versa, due to clear interface boundaries.
- **Clean Code and Readability:** We adhere to PEP 8 style guidelines for Python, ensuring consistent naming conventions and formatting. Variables and functions will have descriptive names (e.g., `buoyant_force` instead of `bf`), making the code self-documenting. We will refactor aggressively to remove duplication and improve clarity, guided by principles like DRY (Don't Repeat Yourself) and SOLID design where applicable in Python.
- **Documentation:** Comprehensive documentation will accompany the code. This includes:
 - Docstrings for all public classes, methods, and functions explaining their purpose, parameters, and return values.
 - An **API reference** document (which can be auto-generated using Sphinx or pydoc) so developers know how to use each module.
 - A **user manual** (possibly in Markdown or as part of a Wiki) describing how to install and run the simulator, and how to use the UI features. This will also explain the physical models and assumptions so that users understand the simulator's scope and limitations.
 - In-code comments for complex logic, especially in mathematical computations, to explain the approach or cite references (e.g., if we implement a specific numerical method, we'll comment the formula and source).
- **Version Control and Collaboration:** The project will use Git for version control. We will maintain a clear commit history and use feature branches for large additions (e.g., a branch for "nanobubble-module" development). Pull requests will be reviewed by peers to ensure code quality and catch issues early. This process also helps maintain uniform coding style and understanding across the team.
- **Testing and Verification:** A suite of unit and integration tests will be developed alongside the code. Some examples:
 - Unit tests for physics functions (e.g., test that `compute_buoyant_force` returns expected value for a given volume and fluid density).
 - Tests for extreme cases (e.g., zero gravity or zero fluid density to ensure code doesn't divide by zero or such).

- Integration test where we run a short simulation and verify conservation laws (for instance, energy input vs output over a cycle within tolerance).
- We will use continuous integration (CI) tools to run tests on each commit, ensuring nothing breaks as new features are added.
- Additionally, validation against real data (if available) or published results will be done. For example, if a paper provides the performance of a KPP at certain specs, we simulate those specs and compare results.
- **Error Handling:** Anticipate and handle possible errors or bad inputs gracefully. If the user enters an out-of-range value (like a negative volume or extremely high number of floaters), the UI will validate and the backend will double-check. In case of a runtime issue (e.g., solver divergence, or OpenFOAM not found), the software will catch exceptions and present a helpful error message to the user ("Simulation unstable due to too large time step – try reducing step size" or "CFD module not available – please install OpenFOAM"). Logging of errors will also be done for debugging.
- **Performance and Profiling:** Use profiling tools (cProfile, line_profiler) to monitor performance hotspots, especially after major additions. Optimize only where necessary – we balance clarity with performance, meaning we won't prematurely micro-optimize clean Python code unless profiling shows a bottleneck. In critical sections identified, we may use techniques like NumPy vectorization, Numba JIT compilation, or rewriting in C++ (with Python bindings) for speed. All such changes will be tested to ensure they don't alter the physical correctness.
- **Plotting and Data Visualization:** Plots generated (either internally or for user export) will adhere to good visualization practices: labeled axes (with units), legends, and captions where appropriate. The color schemes and chart types will be chosen for clarity (for instance, distinguishing multiple floaters by color or line style in a graph). We will also ensure that the visualization does not mislead – e.g., axes starting at zero for meaningful comparison, time axes in proper scale, etc.
- **Scalability and Maintainability:** As the project grows, maintain a clear architecture. We'll periodically review and *refactor* the code to reduce complexity. For instance, if a single function grows too large or a class has too many responsibilities, we'll break it down. We also keep an eye on scalability: if someday someone wants to simulate 100 floaters or run the simulation for hours, is our architecture ready? We design with such future use in mind, using data structures and algorithms that scale (avoiding $O(n^2)$ where n is number of floaters, if possible, etc.).
- **Collaboration and Knowledge Sharing:** The team will maintain an internal wiki or documentation site for sharing knowledge about the project: e.g., explaining the physics models in detail, known issues or limitations, and guidelines for contributing. New team members should be able to read that and ramp up quickly.
- **User Feedback Loop:** Finally, we incorporate feedback from end-users (the engineers using the simulator) continuously. If they find the UI confusing or the simulation results unclear, we address those promptly. This might not be a "coding" best practice, but it ensures the final product truly meets the needs of a high-performance engineering team.

By following these best practices, we aim for a codebase that not only achieves its technical goals but is also sustainable in the long term. Future developers should find it straightforward to add a new module or update an algorithm, thanks to clear structure and documentation. The combination of rigorous testing, documentation, and modular design will result in a **professional-grade** simulator that inspires confidence in both its users and maintainers.

Sources:

1. WELSIM Simulation Software Architecture – Designing modern simulation software emphasizes real-time interactivity, modular multi-physics coupling, and AI integration ¹¹ ¹² ¹³ . These principles guided our architecture and feature roadmap for the KPP simulator.
2. *Collegeboard AP Physics Revision Notes* – Provided the fundamental equations for buoyant force and drag force used in our physics model (Archimedes' principle and quadratic drag) ¹ ² . These ensure our core physics achieve high fidelity.
3. Nature Nanobubble Research – Evidence that nanobubbles at interfaces create a low-viscosity layer, reducing drag in fluids ⁸ . This supports our H1 module design where nanobubbles improve system efficiency by lowering fluid resistance.
4. StudySmarter on Henry's Law – Explanation of gas absorption in liquids at constant temperature ³ , underpinning the isothermal absorption (H2) module whereby dissolved air in water is proportional to partial pressure, affecting buoyancy over time.
5. UCF Physics Text – Relationship between torque, angular velocity, and power ($P = \tau \cdot \omega$) ⁴ . This relation is central to modeling the mechanical-to-electrical energy conversion in the KPP generator and ensuring power output is computed correctly from system dynamics.

¹ ² Revision Notes - Interactions Between Fluids and Solids | Fluids | Physics 1: Algebra-Based | Collegeboard AP | Sparkl

<https://www.sparkl.ac/learn/collegeboard-ap/physics-1-algebra-based/interactions-between-fluids-and-solids/revision-notes/91>

³ Henry's Law: Equation & Constant - StudySmarter

<https://www.studysmarter.co.uk/explanations/engineering/chemical-engineering/henrys-law/>

⁴ 10.8 Work and Power for Rotational Motion - UCF Pressbooks

<https://pressbooks.online.ucf.edu/osuniversityphysics/chapter/10-8-work-and-power-for-rotational-motion/>

⁵ ⁶ ⁷ ⁹ ¹⁰ ¹¹ ¹² ¹³ Design and architecture of modern general-purpose engineering simulation software | by WELSIM | Quantify the Uncertain | Medium

<https://getwelsim.medium.com/design-and-architecture-of-modern-general-purpose-engineering-simulation-software-c923809a66cf>

⁸ Nucleation processes of nanobubbles at a solid/water interface

<https://www.nature.com/articles/srep24651>