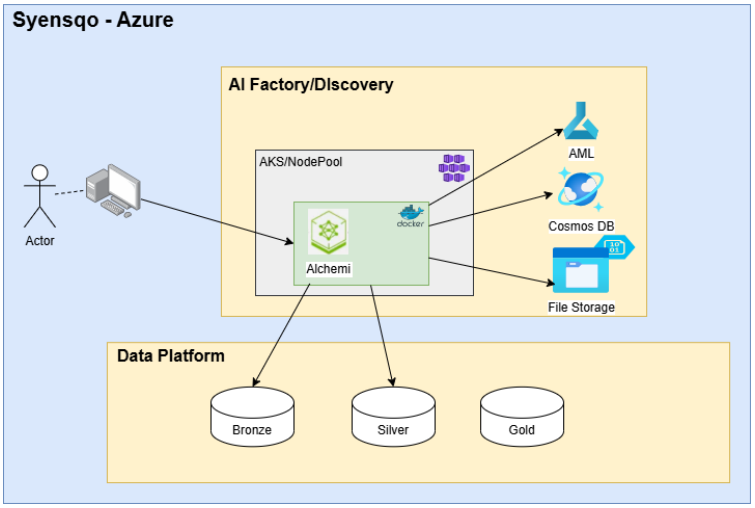
ALCHEMI

1. Technical Capabilities

High Level Design Architecture

General Purpose



A. Architecture & Deployment

- **Containerized Microservices:** Delivered as Docker containers, enabling rapid deployment on GPU infrastructure.
- **RESTful API:** Schema-driven HTTP endpoints for seamless integration with laboratory informatics systems (LIMS, ELN, workflow managers).
- **High Throughput & Batching:** Dynamic batching for efficient GPU utilization, supporting large-scale, concurrent workloads.
- **Async/Agentic Workflows:** Supports high-volume, asynchronous request patterns for automated pipelines.
- **Operational Simplicity:** Configurable via environment variables; minimal setup required.

B. Chemistry & Materials Simulation Workflows

- **Batched Geometry Relaxation (BGR):** High-throughput, batched geometry optimization for molecules and materials.
- **Batched Molecular Dynamics (BMD):** High-throughput, batched MD simulations, supporting NVE, NVT, and NPT ensembles.
- **Periodic & Non-Periodic Systems:** Full support for periodic boundary conditions (PBC) and isolated systems.
- **Cell Optimization:** Variable-cell optimization for periodic systems, with per-request overrides.
- **Partial Optimization:** Per-atom active masks for selective optimization.

C. Machine Learning Interatomic Potentials (MLIPs)

- **Supported Models:** MACE, AIMNet2 (multiple variants), TensorNet, and user-supplied custom models.
- **DFT-D3(BJ) Dispersion Correction:** Optional, for improved van der Waals interactions.
- **Implicit Solvation:** AIMNet2-CPCM variant for implicit solvent effects.
- **External Electric Fields:** Can apply during MD simulations.
- **Custom DFT-D3 Parameters:** User-supplied damping parameters.

D. Data Handling & Integration

- **Input Formats:** Standard chemistry/materials formats via ASE (CIF, XYZ, extXYZ, etc.).
- **Batch Processing:** Multiple structures per request (BGR); single system per request (BMD).
- **Metadata Support:** User-provided metadata fields in requests and replies.
- **Rich Output:** Optimized structures, MD trajectories, energies, forces, stress, charges, and metadata.

E. Configuration & Customization

- **Server Configuration:** Model selection, batch size, DFT-D3 enable/params, cell optimization, tolerances, and more via environment variables.
- **Per-Request Overrides:** Force/pressure tolerances, cell optimization, active masks, etc.
- **Automatic Batch Size Estimation:** Benchmarks optimal batch size based on GPU and memory.

F. Simulation Control

- **Ensembles:** NVE, NVT, NPT with Langevin thermostat and Monte Carlo barostat (including anisotropic).
- **Restartable Simulations:** Long MD runs can be chunked and resumed.
- **Advanced Controls:** External fields, DFT-D3, implicit solvation, custom models.

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2. User Capabilities

A. Workflow Integration

- **Python Client Scripts:** Provided for both geometry optimization and MD, with async and restart support.
- **Command-Line Utilities:** For server readiness checks, batch submission, and workflow control.
- **Example Datasets:** For molecules and materials, periodic and non-periodic, to facilitate onboarding and benchmarking.

B. Informatics Integration

- **Schema-Driven Requests/Replies:** Detailed control over all simulation parameters and metadata.
- **OpenAPI Schema:** For programmatic integration and validation.
- **Health & Status Endpoints:** For monitoring and orchestration in automated pipelines.

C. Usability & Extensibility

- **User Metadata:** Enables traceability and data provenance.
- **Custom Models & Parameters:** Extensible to user-supplied MLIPs and simulation settings.
- **Batch and Async Processing:** Scales to high-throughput screening and automated discovery workflows.

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3. Summary Table

Area	Capabilities
Deployment	Docker containers, GPU-accelerated, ENV VAR config
API	RESTful, JSON schema, OpenAPI, health/status/config endpoints
Models	MACE, AIMNet2 (variants), TensorNet, custom models
Workflows	Batched geometry optimization, batched molecular dynamics

Chemistry Support	Periodic/non-periodic, cell optimization, DFT-D3, implicit solvation, external fields
Batching	Dynamic, auto-tuned batch size, high throughput
User Control	Per-request overrides, active atom masks, metadata, restartable MD
Integration	Python scripts, standard file formats, schema-driven, suitable for informatics pipelines
Output	Optimized structures, MD trajectories, energies, forces, stress, charges, metadata

4. Chemistry-Informatics Perspective

- **Designed for Integration:** RESTful, schema-driven API and standard file formats enable plug-and-play with existing informatics infrastructure.
- **High-Throughput Automation:** Batch and async processing support large-scale virtual screening and automated discovery.
- **Traceability & Data Management:** Rich metadata and provenance features align with best practices in scientific data management.
- **Extensible & Customizable:** Open to new models, simulation settings, and advanced workflows.

5. Benchmarking

Feature capabilities comparison ALCHEMI vs Syensqo Portfolio

Application Mod&Sim Syensqo Portfolio	Overlapping Features with NVIDIA ALCHEMI	Chemistry Use Case Example
Materials Studio	DFT calculations (CASTEP, DMol3); Molecular dynamics; Structure optimization; Crystal builder	Catalyst design; Polymer property prediction; Crystal design
Schrödinger Desmond	GPU-accelerated MD; Free energy perturbation (FEP); Enhanced sampling; REST API integration	Drug-target binding; Protein dynamics; Membrane simulation
Turbomole	DFT; Geometry optimization; RI methods; TDDFT; Large molecule calculations	Excited state chemistry; Reaction mechanism studies
MEDEA / VASP	Periodic boundary conditions; Surface modeling; DFT; Geometry optimization; MD	Heterogeneous catalyst design; Crystal structure prediction
Gaussian	DFT; Hartree-Fock; Geometry optimization; Vibrational analysis	Reaction mechanism studies; Molecular property prediction
CASTEP (MSI)	Plane-wave DFT; Geometry optimization; Phonons; Band structure	Solid-state NMR; Crystal structure prediction
Quantum ESPRESSO	DFT with plane waves; Band structure; Phonons; Geometry optimization; Periodic systems	Battery electrode materials; Catalyst surfaces
COMSOL Multiphysics	Chemical reaction engineering; Electrochemistry; Multiphysics simulation; API integration	Electrochemical cell design; Reactor transport
Aspen Engineering Suite	Batch and continuous process simulation; Thermodynamics; Reaction engineering; API support	Process flowsheet design; Distillation column simulation
gPROMS Process Builder	Dynamic simulation; Equation-oriented modeling; API integration	Complex reaction kinetics; Crystallization
modeFRONTIER	Multi-objective optimization; Simulation workflow automation; API integration	Chemical process optimization; Design space exploration
LAMMPS	Classical and ML-based molecular dynamics, high-throughput, periodic/non-periodic, custom force fields, Python API.	Widely used for materials and molecular simulation, supports integration with ML potentials (e.g., DeePMD-kit).

Feature capabilities comparison ALCHEMI vs Potential other vendor solutions

OpenMM

- **Features:** GPU-accelerated molecular dynamics, Python API, custom force fields, high-throughput, batch processing.

- **Reference:** OpenMM documentation
- **Industry Use:** Drug discovery, protein simulation, supports ML potentials.

ASE (Atomic Simulation Environment)

- **Features:** Python framework for setting up, running, and analyzing atomistic simulations; interfaces with DFT, MD, and ML codes; batch processing; workflow automation.
- **Reference:** ASE documentation
- **Industry Use:** Materials discovery, high-throughput screening.

DeepChem

- **Features:** ML for chemistry, molecular property prediction, integration with simulation workflows, Python API.
- **Reference:** DeepChem documentation
- **Industry Use:** Drug discovery, materials informatics.

Schrödinger FEP+

- **Features:** GPU-accelerated free energy calculations, REST API, batch processing, integration with informatics.
- **Reference:** Schrödinger FEP+
- **Industry Use:** Drug discovery, protein-ligand binding.

ORCA

- **Features:** DFT, semi-empirical, and ab initio calculations; geometry optimization; periodic systems; scripting interface.
- **Reference:** ORCA documentation
- **Industry Use:** Quantum chemistry, catalysis, materials.

6. References

NVIDIA ALCHEMI BGR and BMD NIM Release 1.4

Github repository https://github.com/NVIDIA/nvalchemi-toolkit-ops/tree/main