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SI2: Software infrastructure that ENables Knowledge Integration for modeling coupled geochemical and geodynamical processes

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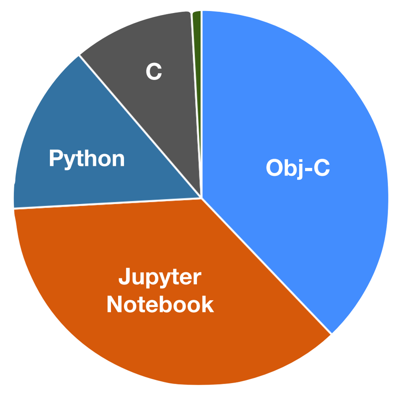
Software Framework



The ENKI software ecosystem aims to provide:

- a central platform for access to models and data - interactive Jupyter notebooks
- a consistent and standardized APIs for coded models
- consistent and standardized interfaces to underlying databases
- a mechanism for building model connections and complex model scenarios - model workflows
- a mechanism for documenting model development and model usage to address the goal of both replicable and reproducible science
- a mechanism for publication and sharing of models and calculations that are based on models or combinations of models

The principal ENKI API is the ThermoEngine Python package, which provides an interface to compiled libraries that implement thermodynamic property retrieval and computational thermodynamics algorithms. Modules include:

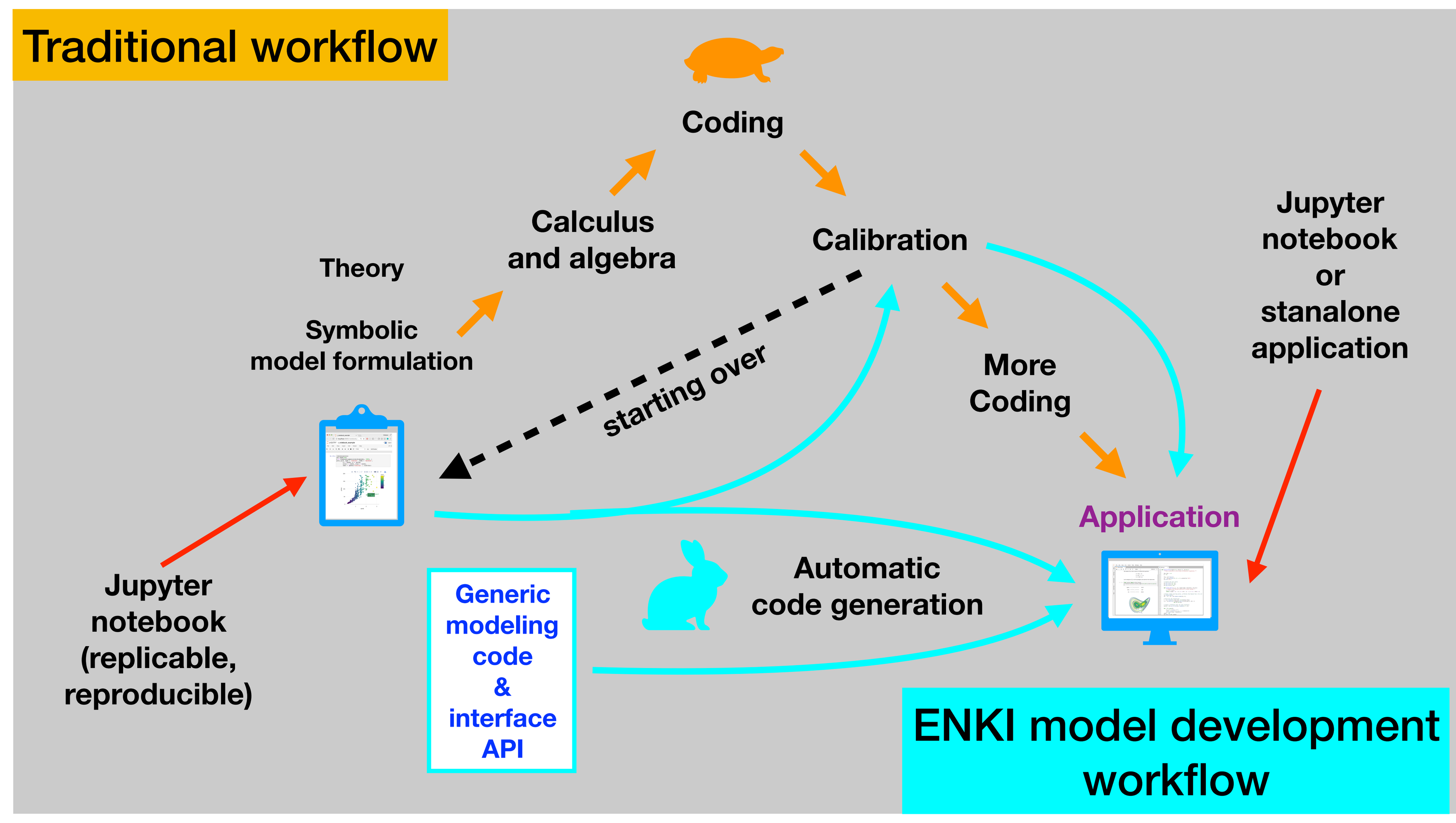
- **calibrate** - provides methods for supporting thermodynamic model calibration using modern Bayesian statistical methods; provides tools to interface with properties and experimental phase equilibrium databases; implements an architecture for replicable calibration and provides visualization and statistical tools for calibration assessment
- **coder** - provides methods for construction of thermodynamic models using symbolic mathematical expressions and for automated generation of expressions for derivative thermodynamic properties and for source code implementation; generates "C" code for inclusion in the phases module and C++ code for generation of computational libraries that support fluid dynamical modeling software
- **core** - provides an interface to our legacy objective C code base and implements generic compositional transformation routines
- **equilibrate** - provides methods that implement equilibrium calculations, including generic equilibrium calculators for Gibbs free energy, Helmholtz free energy, enthalpy and entropy minimization as well as open system calculations; MELTS; speciation models (DEW); equilibrium calculators for systems missing an omnicomponent phase; phase diagram and pseudo section generators
- **graphics** - provides methods for graphical display of properties and phase diagrams
- **model** - methods for loading legacy databases and coder generated model implementations; convenience methods for accessing reaction-based functions; integrated with the phases module
- **phases** - methods implementing a uniform standardized API for accessing thermodynamic properties of pure phases and solution phases; tightly integrated with the model and coder modules

Important URLs

website: enki-portal.org, gitlab.com/enki-portal
server: server.enki-portal.org, enki-ofm-research.org
twitter: EnkiPortal

What is ENKI?

ENKI is a collaborative model configuration and testing portal whose aim is to transform research and education in the fields of geochemistry, petrology and geophysics. ENKI provides software tools in computational thermodynamics and fluid dynamics. It supports development and access to thermochemical models of Earth materials on a Jupyter server platform via Python-based APIs, and establishes a standard infrastructure of software libraries that permit these models to be integrated into fluid dynamical transport codes.



Why is ENKI needed?

ENKI allows scientific questions to be answered by quantitative simulations that are presently difficult to impossible because of the lack of interoperable software frameworks. ENKI modernizes how thermodynamic and fluid dynamic models are used by the Earth science community in five fundamental ways: (1) provenance tracking enables automatic documentation of model development and execution workflows, (2) software tools assist users in updating thermochemical models as new data become available, with the ability to merge these data and models into existing repositories and frameworks, (3) automated code generation eliminates the need for users to manually code library modules, (4) visualization tools and standard test suites facilitate validation of model outcomes against observational data, (5) collaborative groups share and archive models and modeling workflows with associated provenance for publication, (6) "container" publication of Jupyter notebooks and associated software facilitates replicability and reproducibility of scientific workflows.

Modeling tools circumscribed by ENKI