

SI2-SSI: Collaborative Research: ENKI: Software infrastructure that ENables Knowledge Integration for modeling coupled geochemical and geodynamical processes



ACI-15-50482



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Web:enki-portal.org

Project conceptual framework

What is ENKI?

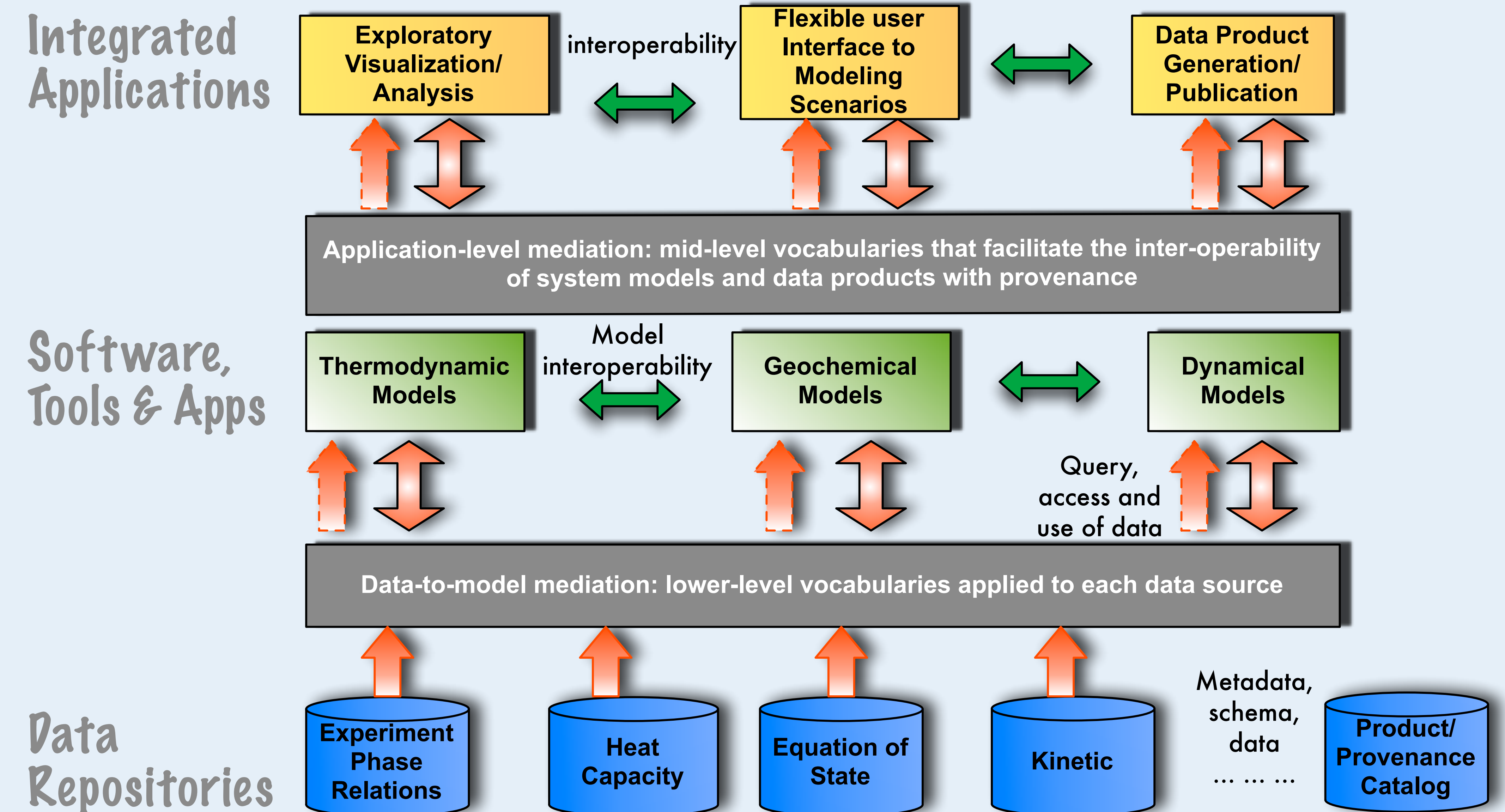
ENKI is a collaborative model configuration and testing portal whose aim is to transform research and education in the fields of geochemistry, petrology and geophysics. ENKI provides software tools in computational thermodynamics and fluid dynamics. It supports development and access to thermochemical models of Earth materials, and establishes a standard infrastructure of web services and 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 will enable automatic documentation of model development and execution workflows, (2) new tools will 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 will eliminate the need for users to manually code web services and library modules, (4) visualization tools and standard test suites will facilitate validation of model outcomes against observational data, (5) collaborative groups will be able to share and archive models and modeling workflows with associated provenance for publication.

Project status - month 5 of a 36 month effort

- Assembled and prioritized modeling software for porting and repackaging; ported several thermodynamic data/model collections and exposed these as library frameworks (C, C++, Objective-C, with python wrappers)
- Initiated a documentation project for library APIs; developed website; converted course instructional materials into Jupyter notebooks
- Installed a Jupyter server for testing and deployment of python and R notebooks
- Began development of Jupyter notebooks that will be used to access model frameworks and provide visualization tools for model outcomes
- Began development of software tools for model calibration and maintenance
- Began accumulation of literature data for inclusion in data repositories
- Invited early career participants to workshop; scheduled workshop and venue; planing workshop activities
- Convened workshop (sponsored by CIDER; Jan 25-27) to explore API and data communication between CT and CFD modeling software



Project implementation timeline

Year	1	2	3
Workshop participants	objectives & prioritize needs	(alpha/beta testers)	evaluate; refine; educate (beta testers)
Extant software	selection & porting	web service development	documentation and web UI
Data collections	specification of schema	community input -> refine	populate data collections (DCO activity)
Model Interoperability	propose schema in consultation with CIG & COMPRES	develop prototypes	use cases & documentation
Model user interface	Prototype from ThermoFit	develop capabilities	port to web platform
Model calibration tools	extant model porting/data source integration	UI integration & visualization	Bayesian & Monte Carlo methods
Model forward visualization	extant model visualization	development	integration with UI, visualization & calibration feedback capability
Model codegen & web services	develop specifications	Code automatic code generation/ UI/web services	refinement
Model test suites & certification	develop extant model unit tests	Integration with UI	documentation
Model self documentation	develop specifications	Integration with UI	archival/publication
Model social networking	develop specifications	Integration with UI	refinement
Instructional materials	Consolidation and organization of extant materials	Development of new exercises and tutorials based on the new UI	refinement

Responsibility: ■ Ghiorso ■ Fox ■ Bergantz/Spiegelman ■ Shock/Sverjensky ■ All PIs