Next Generation Cyberinfrastructure for Geochemistry & Petrology: Connecting Data (EarthChem) and Models (ENKI)

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Research in geochemistry, volcanology, and petrology is evolving to more data-driven and computational approaches. Such methodologies increasingly rely on access to large volumes of geochemical and petrological data as well as computational environments for modeling natural systems. Use of Machine Learning, Monte Carlo simulation, and other data science methodologies is emerging as a new modeling paradigm, and existing computational and data resources need to evolve to support these novel research workflows. EarthChem maintains and provides access to large-scale global syntheses of geochemical measurements of natural specimens and experimental data (LEPR, traceDs) and is currently in the process of modernizing its architecture and services to respond to evolving requirements for machine access (APIs). ENKI is a collaborative model configuration and testing portal that provides software tools in computational thermodynamics and fluid dynamics and facilitates development and access to thermochemical models of Earth materials. EarthChem and ENKI have started a joint effort to develop the next generation cyberinfrastructure for geochemistry and petrology that will connect EarthChem's databases to the ENKI modeling environment. This updated system will allow the community to build and calibrate models, provide access to the models for the purpose of validating the models of others, establish new data analysis and visualization tools, and apply these tools to natural systems. The EarthChem-ENKI modeling environment will be made available via open source Python frameworks, and community access will be afforded using containerized cloud-based services.