Virtual Research Environment Integrating Heterogeneous Data Resources for Materials Science and Engineering

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Abstract: Materials performance analysis process requires integration of many heterogeneous data and information resources, e.g. experimental data, empirical models and computational simulation. Virtual Research Environment (VRE) for materials science and engineering should support each data handling processes, data retrieval, conversion, statistical analysis, symbolic manipulation and visualization within single interactive and scripting environment.

Furthermore, in order to integrate heterogeneous data, it requires a common dictionary which describe semantic relationships among these data resources. It is required to identify corresponding data items from different data resources. It can be a flat structured table, but an ontology which describes semantic relationships among concepts, is much preferable

Scripting language Python provides many of these capabilities with additional software modules and widely applied for interactive/non-interactive data processing environment. In this presentation, a prototype design and implementation VRE for materials science and engineering based on SageMath open source mathematics software and examples of ontology utilization for materials data integration.