the ENERGY lab

PROJECT FACTS

Advanced Research

Materials- Design of Multiscale Systems

Background

The U.S. Department of Energy (DOE) promotes the advancement of computational capabilities to develop materials for advanced fossil energy power systems. The DOE's National Energy Technology Laboratory (NETL) Advanced Research (AR) Program is working to enable the next generation of Fossil Energy (FE) power systems. The goal of the AR Materials Program is to conduct research leading to a scientific understanding of high-performance materials capable of service in the hostile environments associated with advanced fossil-fuel based power production.

NETL has teamed with the DOE's Ames Laboratory to develop tools capable of integrating materials design into the overall technology design process. A basic challenge in materials design is the need to address a wide range of scale-related effects and their interactions, from electronic structure to dislocations or grain boundaries. Usually, these different scales are studieded by different research or design teams, but this project will develop an integrated approach to exploit additional degrees of freedom in the design space.

Project Description

The aim of this project is to develop the computational algorithms and strategies needed to design materials across dimension and time scales, creating the ability to design and tailor material properties for specific applications. Success will enable not only the development of new materials but a true integration of materials design as part of the product design process.

The overall approach of the project will focus on the following four areas: (1) development of a deeper understanding of information flow in a multiscale materials system; (2) development of mathematical descriptions and algorithms needed to describe the flow of that information; (3) implementation of these mathematical algorithms into engineering software tools; and (4) application of those tools to describe and design optimal materials for energy applications.

The work will be accomplished through the completion of five (5) technical tasks. Task 1 will create a shared vocabulary to facilitate understanding about how information is connected in a multiscale system. Task 2 will assess the capabilities of computational methods and models across a multitude of scales and will identify those methodologies most likely to be successful when scaled up to the complexity of a multiscale computational framework. Task 3 will involve the development of an open-source library of tools that implement the previously selected algorithms into a multiscale design framework (VE-Suite). Task 4 will develop test cases to demonstrate proof of principle for the methods and linkages developed into VE-Suite. Task 5 will develop design tools to optimize materials properties as part of an overall product design.

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PROJECT DURATION

Start Date
04/01/2010

End Date
09/30/2011

COST

Total Project Value
$180,000

DOE/Non-DOE Share
$180,000 / $0

Goals/Objectives

The aim of this project is to develop the computational algorithms and strategies needed to design materials across length and time scales, creating the ability to design and tailor material properties for specific applications.

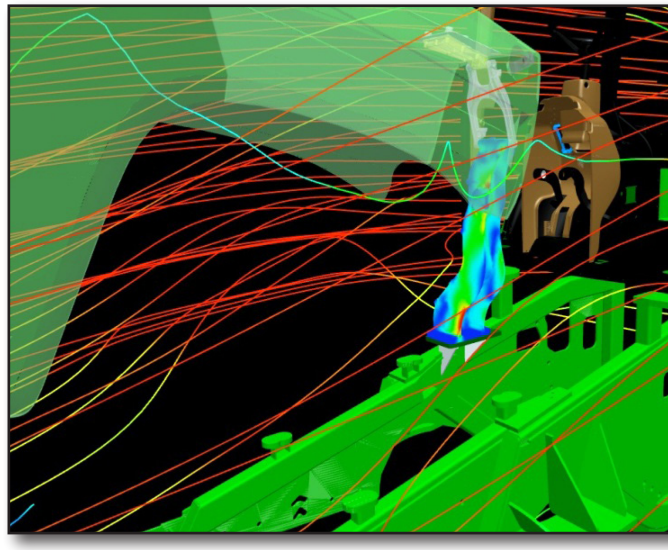
Accomplishments

An information flow map was developed for multiscale materials simulation.

Specific software codes that will be implemented within VE-Suite were identified, and the main high temperature materials classes for focus in this project were selected.

Benefits

Engineered designs are generally based on the use of a constrained, and fixed, set of materials. However, as multiscale materials behavior is understood, researchers will be able to design the material properties of each part, providing more flexibility in the design of new materials. This project will enable not only faster development of new materials but the possibility of a true integration of materials design as part of the product design process.



Graphical output from VE-Suite of a simulation of the response of a part to an external load