TITLE: Computer Scientist / Materials Scientist
DEPARTMENT, AGENCY: Department of Energy, National Energy Technology Laboratory
STIPEND RANGE: Depends on level of experience
OPEN PERIOD: Open until filled
LEVEL: Post-Doc
POSITION INFORMATION: Temporary Appointment: 1 year starting period between Oct 1 and Nov 14, 2013; Full-Time (40 hours per week).
WHO MAY BE CONSIDERED: United States Citizens; Foreign Nationals holding F-1 Visa with OPT & EAD Card, or J-1 Visa status inside the US, and LPRs

DESCRIPTION:

An opportunity exists for a post-doctoral researcher or a visiting scientist at the PhD level to develop computational models and data analysis tools in support of the NETL Solid Oxide Fuel Cells research group. Research efforts focus primarily on: (1) accurate capture of the relevant physical processes; and (2) validation of models using detailed in-house experiments or independently published reports. Within individual model development tasks, a lower priority has been assigned to ensure that the models and tools are computationally efficient, widely accessible, and share data. This position will provide support directly to collaborators to transfer existing models to the High Power Computing (HPC) platform known as the SBEUC, operate the codes to ensure accurate results are being obtained in the new environment, and begin to place user interfaces on models to facilitate broader accessibility. Broadly, the project goals are:

1) Generate computational environments using commercially relevant paradigms that allow rapid execution of existing fuel cell models;
2) Establish a user interface for each of the independent models that permits a non-expert to complete simulations;
3) Implement a methodology for data exchange between independent modules, ultimately producing a comprehensive SOFC performance model;
4) Ensure that models are computing in true parallel fashion;
5) Generate high fidelity visualization tools supporting analysis.

SPECIFIC TASKS:

The specifically envisioned tasks support the broad goals described above.

1) Examine existing codes for 5 models to determine the strategy for transfer of codes to HPC. The priority ranking of the code transfer is:
    a. Oxygen Reduction Reaction Model (LSM and LSCF) – PI: Xingbo Liu (WVU); RA: Hui Zhang (WVU)
    b. 3D Multi-Physics Model – PI: Ismail Celik (WVU); RA: Raju Pakalapati (WVU)
    c. Microstructural Evolution Model – PI: LongQing Chen (PSU); RA: Linyun Liang (PSU)
    d. High Fidelity Impedance Model – PIs: Ismail Celik (WVU) & Harry Finklea (WVU)
    e. ** Bayesian Statistical Model – PI: David Mebane (WVU); GA: Joshua Blair (WVU)

    For each model, the incumbent is expected to evaluate whether:
    A. The model should be computed in existing code
    B. The existing model code should be ported to facilitate HPC interaction

    Note that SOFC industry teams prefer the use of FLUENT, so HPC codes will ideally be compatible.

2) Generate stand-alone computational modules that allow rapid computing. Model should contain a user interface that allows manipulation of parameters by a non-expert user. Results generated

using the HPC environment must be compared to those generated via PC, to ensure equivalency of the environments.

3) Generate a method to pass data from one computational module to another, such that results from one model can be used to update the starting parameters in another model. Ensure that the models can all be executed in true parallel form.

4) Generate high quality visualization tools indicating cell performance in time and space. Permit user queries at high fidelity.

5) ** Develop impedance tool to correlate impedance data with physical processes, with high confidence in assignment. The tool will consist of:
    a. Means for importing impedance data
    b. Deconvolution of impedance data
    c. Generation of high fidelity impedance simulation
    d. Generation of equivalent circuit
    e. Optimization routines minimizing errors in assignment of elements, processes, and rates across all analytical methods (b,c, and d).
    f. Fit analysis and visualization

QUALIFICATIONS:

The successful candidate will possess demonstrable skill in advanced mathematical algorithms and computational methods for solving complex reaction and transport problems. The successful candidate will possess significant experience in computer programming, and will preferably have experience in programming suitable for a high power computing environment. The successful candidate will possess excellent communication skills, and will possess demonstrable experience completing research in a collaborative/team environment.

The successful candidate is NOT required to possess experience in solid oxide fuel cells or related materials, but preference will be given to candidates with experience in solid oxide fuel cells, electroceramic materials, electrochemistry, or any related systems in sensors, membranes, and other energy conversion devices.

Interested candidates may contact Dr. Kirk Gerdes (kirk.gerdes@netl.doe.gov) directly with a current CV at the earliest opportunity.

HOW TO APPLY:

Applicants should apply through the Oak Ridge Institute for Science and Education (ORISE) program (orise.orau.gov). NETL utilizes the ORISE program to support research and work within NETL's Office of Research & Development.

• Interested applicants should complete the online application at https://netl.orau.gov/
• In the online **application list Dr. Kirk Gerdes as your requested mentor**. This will associate your application with this job posting.

If you have additional questions please contact the NETL ORISE program coordinator, Nancy Andres, Nancy.Andres@NETL.DOE.GOV.