I. Problem statement:

Our research group is focused on designing, characterizing and gaining a fundamental understanding of new-age advanced materials. To this end, we are currently involved in a number of projects with the following desired outcomes:

- *Design of high strength advanced steels*: the goal is to predict the optimum temperatures for two-step heat treatment to maximize the retained austenite in TRIP steel by employing a three pronged approach – heat treatment design, modeling of plastic flow behavior and it's Bayesian parameter calibration

- *High temperature shape memory alloys (SMAs)*: the focus is on understanding the magnetic and structural transformations, magneto-caloric and elasto-caloric effects, and formation of spins and strain glass in SMAs using first-principles calculations and Monte Carlo.

- *Metallic fuels*: investigate the effect of actinides and fission products on the phase stability of the fuel by studying the electronic structure and phase equilibrium using ab-initio calculations.

- *Lead-free soldering*: investigating the microstructure evolution of intermetallic compound under the effect of orientation, nucleation using phase-field models

- *Materials Informatics and Design*: development of materials database and curator to facilitate materials design. The focus is on SMAs and MAX phases, which promise many interesting and practical applications.

II. Background:

Apart from the collaboration with experimentalists on and off-campus for model verifications, our approaches for the aforementioned projects mainly based on computational efforts. Particular computational techniques that we used in our studies vary from *ab-initio* calculations at the atomic level (VASP) to Monte Carlo (MC) and Molecular Dynamics (MD) at the meso- scale to phase field modeling (PFM) at the continuum level using in-house parallel Fortran codes as well as uncertainty analysis based on Markov Chain Monte Carlo (MCMC) using commercial Matlab software. Details on these computational approaches and justification for their SU applications are listed in the following sections.

As we have experienced, most of these calculations are expensive and have to be performed either with many computer nodes (VASP) or in a long duration of time (MCMC) or both (PFM, MC). We find that

ADA is very efficient in terms of queue time, number of jobs, runtime speed, and cluster stability. This appears to be comparable or even better (in terms of queue time and number of job) than the TACC cluster, according to our experience. We therefore find that ADA is crucial to the success of our projects.

III. Methodology:

For the project that we are currently working on, we utilize computational tools across length scale, in particular:

- *VASP*: a computational package based on first-principles theory (density functional theory (DFT)) for electronic structure calculations at atomic scale. It is used throughout our projects to investigate the effect of electronic structure on the properties of our investigated materials. It can also be used to estimate thermodynamic properties of the materials at ground state (0K or -273^0C) and even at elevated temperatures. These are all expensive calculations.
- *SPRKKR and EMTO-CPA*: apart from VASP, we also use other DFT-based SPRKKR and EMTO-CPA packages for investigation of configurational ordering and magnetic properties of materials. These are parallel codes and can be expensive when the number of atoms per crystal unit cell is high.
- *Phase-field modeling*: an efficient approach to the modeling of microstructural evolutions. We has constructed several phase-field codes using Fortran 90 language. The codes are highly parallel for simulating a large domain of microstructure evolutions. These codes are currently used to investigate lead-free soldering based on Cu-Sn and in the near future Cu-Sn-Ag, solute trapping and rapid solidification of NiTi shape memory alloys during additive manufacturing and microstructure evolutions in metallic fuels for Gen-IV nuclear reactors.
- *Monte Carlo simulations*: Monte Carlo has been successfully used in our group to investigate phase stability/phase diagrams of shape-memory alloys at elevated temperatures. Recently, we also adopt MCMC to assess modeling uncertainty. The MC-based codes developed for these purposes are parallel mainly with OpenMP for spatial domain since the highly parallel MPI is not essentially more efficient due to the time-sequential nature of the simulations.
- *LAMMPS*: Without limited to these tools, we intend to use extend our methodology to other approaches when they come to serve better the purposes and goals of our projects. The current micro-scale tool which we have in mind is LAMMPS, a molecular dynamic package, which can be used to estimate kinetic diffusivity of materials. These diffusivity are important within the context of microstructural modeling such as PFM and MATCAL.

For running all these packages/software for the aforementioned projects, we estimate a total cost of **4,990,080**. Following sections will mention about how we plan to distribute these computer resources according to our research schedule as well as the justification for the requirement.

IV. Research plan:

The research schedules we have for each project this applied fiscal year are listed in this section, as follows:

- Study of lead free soldering using Phase Field Modeling: the plan of this project this year is two folds: first, the electro-migration will be investigated within Cu-Sn microstructural evolution. This phenomenon is believed to reduce the performance of Cu-Sn soldering and therefore the performance of 3D-integrated circuit. Second, the effect of elastic strain on the microstructure evolution of Cu-Sn. Due to the weight of these tasks, we expect ¾ of the applied year for the first task leaving the remaining time to initiate the second task.

- Actinide alloys for Gen-IV Reactors: in this project, the computer resources for 1/3 of the applied fiscal year will be spend to study the electronic structure of the actinide alloys, particularly U-Zr, on its thermodynamic properties using first-principles tools including but not limited to VASP and EMTO-CPA. The following 1/3 of the applied fiscal year will be use to assess the thermodynamics of the U-Zr system using the CALPHAD approach, implemented via the Thermo-Calc and OpenCALPHAD packages. The last 1/3 of the fiscal year, we will spend the applied computer resources on developing/testing a phase-field model for rapid solidification of U-Zr under different thermal gradients.

- Strain glass Project (0.5 Million USD): the task of this project in this year will be investigate the effect of chemical composition, ordering configurations, and magnetic moments on the phase stability and transition of NiCoMnIn-austenite and martensite, using first-principles packages including but not limited to VASP, SPR-KKR, and EMTO-CPA. This is expected to occur within the first half of the applied fiscal year. In the remaining second half, we plan to spend the computer hours on fitting parameters of a Hamiltonian used for Monte Carlo – based estimation of (metastable) phase diagram of NiCoMnIn austenite and martensite phases. This fitting is an inverse Monte Carlo process hence expensive and time consuming. To facilitate this, we plan to try the efficiency global optimization scheme (EGO) to optimize the Hamiltonian parameters on the fly.

- DMREF on High Temperature Materials (1.5 Million USD): the scope of this project is large and including many folds as it covers computational studies of Hf-based shape memory alloys across length scales from atomistic to continuum with verifications from experiments. The task in this year focus on the investigation of thermodynamics (phase stability) of the alloys by means of first-principles calculations, using mainly VASP, and CALPHAD, using Thermo-Calc package. We expect to spend a whole applied fiscal year for this specific task, as the VASP calculations tend to be very expensive as it requires large supercells with many atoms to cover the interesting compositional range. Also, expensive first-principles phono calculations may also be carried out for high temperature energies that are valuable for understanding the thermodynamics of the materials.

- Materials Informatics and Design (3 Million USD): in this project, we will carry out first-principles calculations using our home-made workflow manager, TAMMAL, specifically design to be compatible with ADA. This task will be constantly throughout the applied fiscal year in order to calibrate for the ground-state mechanical and thermodynamic properties of materials,

with focus on shape memory alloys and MAX phases, which are two interesting classes of materials with many practical applications

- **Requirement analysis:**

To justify for the above supercomputing unit we are applying for, the following analyzes the estimated cost of our computation effort upon each project:

- Lead free soldering using Phase Field Modeling
    - Code: Custom PFM, FORTRAN
    - Clusters: Lonestar 5
    - No of SUs per run: 400
    - Estimated no.of runs: 250
    - Total computation cost: 100,000 SU

- Actinide alloys for Gen-IV Reactors
    - Code used: VASP, SPRKKR, EMTO-CPA, phase–field modeling
    - Clusters: Lonestar 5
    - No of SUs per run: 400
    - Estimated no.of runs: 250
    - Total computation cost: 100,000 SU

- Strain glass Project (0.5 Million USD)
    - Code used: VASP, SPRKKR, Custom Monte Carlo Codes, Molecular Dynamics
    - Clusters: Lonestar 5
    - No of SUs per run: 2000
    - Estimated no.of runs: 100
    - Total computation cost: 200,000 SU

- DMREF on High Temperature Materials (1.5 Million USD)
    - Clusters : Clusters: Lonestar 5
    - Code used: VASP
    - Clusters: Lonestar 5
    - No of SUs per run: 2000
    - Estimated no.of runs: 50
    - Total computation cost: 100,000 SU

- Materials Informatics and Design (3 Million USD)
    - Code used: VASP, Galaxy
    - Clusters: Lonestar 5
    - No of SUs per run: 2000
    - Estimated no.of runs: 50
    - Total computation cost: 100,000

Total requested time on ADA therefor is: **600,000 SU**