Allocation Name

WD_VDMF
ITS$-wdn-10000

Title Of Allocation

Framework for Modeling Vascular Damage Caused by Radiation – Development Allocation

PI

Wayne Newhauser

Research Categories

Biophysics
Software Development

Description of Research

Increasing patient survival rates following cancer treatment have brought more attention to the long-term effects of radiation therapy, which can detrimentally affect the patient's quality of life. Radiation-induced necrosis of the brain has received increased attention in the literature due to the difficulty of diagnosis, its severe and potentially deadly impact on the patient's quality of life, and concerns over its relation to proton and heavy ion therapies. Researchers have demonstrated a correlation between vascular network damage and necrosis induction. The long term goal of this project is to investigate the mechanisms linking vascular damage to radiation induced necrosis through simulation and small animal models.

Vascular networks in an organ, such as the brain, contain billions of vessels with dimensional scales spanning four orders of magnitude. The calculation of dose to large multi-scale geometries is computationally difficult and time consuming. Recent improvements in the modeling of vascular network geometry and radiation track structure lend themselves to the investigation of multi-scaled damage in vascular networks of a human brain. However, the computational requirement such a model for the whole brain poses one of the biggest challenges. The goal of this project is to develop a computational framework for simulating vascular radiation damage, and to show that it is computationally feasible to perform these calculations for the whole brain.

To investigate the role of multi-scale vascular damage in radiation-induced necrosis, we will develop a computational framework to simulate radiation damage on whole-organ vascular networks. Using this framework, we will test the following hypothesis: *It is computationally feasible to simulate multi-scale radiation-induced changes with 10% statistical uncertainty in a 3 billion vessel network, mimicking the human brain, within 3 million CPU-h using less than 4000 CPUs.*

We propose to the test this hypothesis by performing the following specific aims:
Specific Aim 1: Evaluate a computational figure-of-merit (composite of accuracy, speed, and efficiency) for multi-scale dose calculations of proton tracks incident on a vascular network, while limiting simulation time to 2 million CPU-h ($FOM \geq 5 \times 10^{-5}$).
Specific Aim 2: Determine if multi-scale simulations of vasculature shrinkage caused by radiation-induced DNA damage can be completed in 800,000 CPU-h for the entire brain vascular network.
Specific Aim 3: Determine if changes in blood flow through the whole-brain vascular network can be computed using steady state Poiseuille equations within 200,000 CPU-h using less than 512 GB electronic memory.

The requested allocation will be used to perform debugging and initial scalability tests for the major application sections. The scalability demonstrated here will be used as preliminary results for a Research Allocation of LSU HPC resources and XSEDE resources if necessary. Additionally, some results will be used in the publication of manuscripts based on the thesis work. Finally, initial scalability testing can be used in abstracts for conference presentations. This allocation will have about 10,00 SUs dedicated to debugging, 10,000 dedicated to scalability testing, and the remainder used for Preliminary Results generation.

Is research commercial?

No

Description of code (1 paragraph)

The code used in this project is being developed by a graduate student for his Ph.D. Dissertation project. The software framework can be broken into 5 major software applications: vascular network creation, partitioning, dose calculation, biological modeling, and blood flow modeling. The code is being built C++ using a hybrid architecture. The different aspects of the framework are compute or memory bound. The biggest issue is the memory required to describe the network geometry, connections, and dose information. Currently completed are codes for generating the network and partitioning the network. Code to calculate the blood flow is nearly complete with only a minor communication section needing to be written before it is complete. The code leverages many different libraries discussed below. Parallel I/O is used to improve the throughput of the application.

Code Requirements (compilers, file formats, etc.)

The application uses the following libraries and compilers:
Intel C++ Compiler 2017
Intel MKL 17.0 – Cluster Edition
Intel MPI
HDF5 version 1.10-patch 1
ParMETIS ver. 4.0.3
Google Test

The application additionally uses CMake (ver 3.6) to configure the build environment.

Many of these libraries are not available on Super Mike II or Super Mic. These libraries will be installed and compiled in a project allocation that has been set aside.

The program uses HDF5 as its File I/O library. Using the Parallel HDF5, compression is not an option. Throughout the projects the files will be temporary and can be deleted once the project is complete. It is expected that the largest file size for the entire project will be approximately 5 TB. At the end of each run the file will be removed from the Work directory.

Is code check pointed?

No

Estimate of Resources Needed

4 GB per Proc or 64 GB per node

Most important machine characteristic for the code

Latency is currently worst part.

Allocation Type and Number of SUs

The allocation type requested will be startup and I am requesting 50,000 SUs

Scaling and performance information

Initial scalability and testing for the currently completed applications were performed on a personal desktop with a single 4-core cpu (Intel I5-3570K) and 32 GB of memory. The data shows a slight improvement in performance when adding MPI processes, with a majority of the time being used in the I/O stages. I believe that this will be reduced when a parallel file system is available. I expect better strong scaling when the i/o limitation is removed.

Additionally, the vascular creation and partitioning codes perform excellently. Their projected runtime is expected to be less than 100 SUs each for the largest trails to be run. This is good because it is required for each trial run of the larger applications.

Publications citing resources used at HPC

N/A

Grants awarded and/or pending

N/A

Pending and/or successful applications for computer time at other facilities

N/A