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# **Problem Description**

Current models for simulating the evolution of material defects caused by radiation damage on the microscopic scale take far too long to run, limiting their usefulness.

## **Scope**

The scope of this project will be limited to simulating a particular model of radiation damage called cluster dynamics taking advantage of GPU parallelism. Stretch goals include altering this model using additional methods such as Monte Carlo simulation in order to get more accurate results in a more reasonable time.

## **Use Cases**

The project partner will benefit directly from this project because it will allow them to conduct simulations on a scale previously impractical, speeding up their research.

# **Purpose and Vision (Background)**

Our purpose is to speed up simulations of radiation damage. Research in this area is bottlenecked by simulation speed.

# **Stakeholders**

* Project Partner

The primary decision-maker because they will use this project directly. They will receive updates at least once per week, or more if the engineering team has questions about the product requirements. They require insight from the engineering team to know what is possible with the computational resources we have access to.

* Engineering Team

Will receive updates multiple times per day from other team members, especially as their work affects each other. They will make most of the low-level decisions about the computational aspect of the project. They require insight from the project partner to understand the materials science and physics aspects of the project, along with what would best serve them in a final product.

# **Preliminary Context**

## **Assumptions**

The program we develop should be able to run on Linux and utilize the resources of a GPU in a headless environment.

We will have access to the DGX at OSU for compute resources.

We have about nine months with our engineering team to bring the project to a place that is usable.

## **Constraints**

Exactly what kind of resources we have access to, compute or otherwise, isn’t fully known. We’ll need to do more research as it becomes clearer what our needs will be.

We will need to utilize the GPU for speeding up these simulations, because there’s likely no way to get a significant speedup without relying heavily on parallelism.

We have a low number of engineering hours per week because each of us have other obligations. We can probably realistically expect at most 10 hours of engineering time per week out of each engineer.

## **Dependencies**

Any progress on creating the simulation first relies on the engineering team getting up to speed on the model of radiation damage we’ll be using

# **Market Assessment and Competition Analysis**

More research needs to be done on this front. I suspect there are existing products which could help significantly with the problem. The question is exactly how much a third party program could help when put against the difficulty of just writing a custom simulation.

# **Requirements**

*The requirements will drive your software development. It will give you the big picture of what you’re building, and the whole team should be aware of and agree on it.*

## **User Stories and Features (Functional Requirements)**

More research is needed for the engineering team to understand the use cases - the team is working through a few readings given by the project partner.

## **Non-Functional Requirements**

* Code should be well-documented, following coding standards and best practices.
* The product should be able to scale up for use with large computing resources, such as GPU clusters.

## **Data Requirements**

More research is needed - this will be fleshed out over the next week or two.

## **Integration Requirements**

The program needs to be able to interface with a GPU using CUDA.

## **User Interaction and Design**

More research is needed - this can be figured out after we understand the use cases.

# **Milestones and Timeline**

More research is needed - this can be figured out after we understand the use cases.

# **Goals and Success Metrics**

More research is needed. One idea is:

| **Goal** | **Metric** | **Baseline** | **Target** | **Tracking Method** |
| --- | --- | --- | --- | --- |
| Speedup cluster dynamics simulation | Percent speedup over baseline | TBD [Perhaps whatever program the project partner used previously] | TBD | TBD |

# **Open Questions**

Who will use the simulation? What might they use it for? What results do they require from it?

Are there any existing products which would meet those needs?

What existing methods were used and how did they run into problems?

What kinds of computing resources could we get access to?

How exactly will the simulation work? What kind of data will it track? How will it transform that data?

How parallelizable is the type of simulation that the project partner has in mind?

# **Out of Scope**

Data visualization / analysis may be out of scope for this project. Data visualization is important but the end user may simply need to import the data into a more general-purpose visualization program. More important is formal data analysis, which will also likely not fall within the project scope. The end product will likely be a command-line program.