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Estimating Z-Pinch Computing Resources

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Abstract

The Z facility at Sandia National Laboratories produces high energy density environments. Computer simulations of the experiments provide key insights and help make the most efficient use of the facility. This document estimates the computer resources needed in order to support the experimental program. The resource estimate is what we would like to have in about five years and assumes that we will have a robust, scalable simulation capability as well as enough physicists to run the simulations.

Acknowledgments

Many people have contributed to this document, suggesting editorial changes, helping provide the computing estimates, or providing the background of why the simulations are needed in the first place. These people are: Thomas Mehlhorn, Raymond Lemke, James Ang, and Michael Desjarlais.

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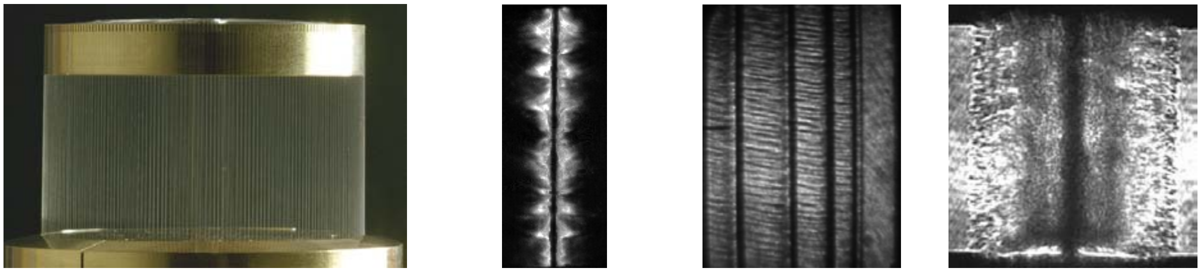
1 Introduction

The Z facility at Sandia National Laboratories produces high energy density environments used to support several Science Campaigns. Campaign 4 (Secondary Assessment Technology) and Campaign 7 (Nuclear Survivability) experiments are driven by radiation from Z-pinches. Campaign 2 (Dynamic Materials Properties) experiments study the equations of state for various materials under extreme shock conditions. But the primary focus of the Z facility is Campaign 10 work, Inertial Confinement Fusion (ICF).

Tight integration of a modeling and simulation capability with the experimental program increases the effectiveness and impact of the Z facility for the Science Campaigns. Estimating the necessary computing resources to support an experimental program is important, but is always difficult. There are large uncertainties and variabilities to the complexity of the required simulations, the availability of analysts to perform simulations, and the computational power of future systems.. The estimates in this document assume that we have enough analysts to do all the simulations that we would like to do to support the experimental program. We have a successful predictive capability in order to support the Campaign 2 work, and these estimates extrapolate the needs of that capability to the more challenging Z-pinch design work. The computational and science challenges unique to Z-pinch ICF are explored below, but the needs of ICF capsule design are also important to the program. In fact, the usage estimates include both Z-pinch and ICF capsule design work.

All processor-hour estimates are normalized to Purple processors (IBM POWER5), and no attempt has been made to estimate the increase in processor speed. This is worth mentioning because 512 processor simulations that are typical today were unimaginable five years ago, even if we had unlimited time on a large capability systems available at that time.



(a) 10 μm diameter wires arranged in a 2 cm cylinder.

(b) A single wire initiates.

(c) Several wires ablate inward.

(d) Entire array stagnates on axis.

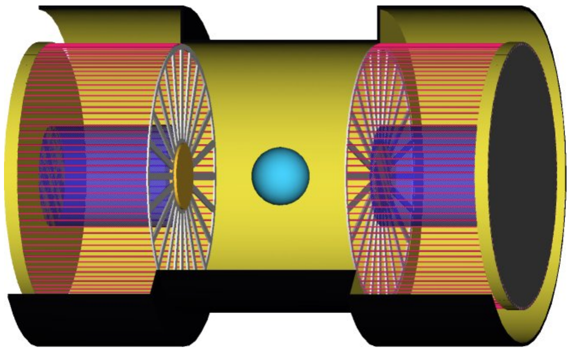
Figure 1. A 19-26 MA current is applied to an array of several hundred 10 μm diameter wires. The wires heat and ablate plasma. The plasma is driven inward by the magnetic field and stagnates on axis, generating an intense radiation pulse.

2 Physics of Z-Pinch Implosions

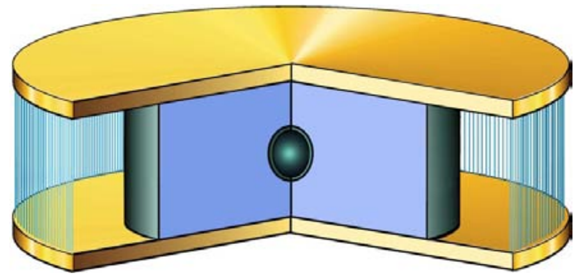
Z-pinches convert a large electrical current to an intense radiation pulse[3]. Figure 1 shows the different phases of a Z-pinch implosion. On Sandia National Laboratories' Z facility, hundreds of 10 μm diameter wires, Figure 1(a), are arranged in a cylinder that is about 2 cm in diameter. A 19-26 MA current run through the wires over 100 ns delivers about 3 MJ to the pinch. As the wires heat, they ablate plasma, Figure 1(b). The strong magnetic field that develops around the array pushes the plasma inward, seen in Figure 1(c). Eventually the wires are completely ablated, the array implodes, and the plasma stagnates on axis, Figure 1(d). The kinetic energy of the stagnating plasma is rapidly converted to thermal energy, generating an intense radiation pulse.

The radiation pulse can be tailored by changing details of the pinch[1, 2]. The type of material used for the wires changes the spectrum of the radiation. Pulse shaping can be achieved by inserting foam targets on axis, by varying the mass of the array, and by nesting two wire arrays.

Figure 2 shows two different designs for driving ICF capsules with Z-pinches. In a Doubled-Ended Hohlraum, Figure 2(a), radiation from two Z-pinches drive a capsule in a secondary hohlraum. The capsule in a Dynamic Hohlraum, Figure 2(b), is driven by a radiating shock in the foam generated by the collision of the Z-pinch.



(a) In the Double-Ended Hohlraum, radiation produced by two Z-pinches drive a capsule in a secondary hohlraum.



(b) The imploding Z-pinch collides with the foam, and the subsequent radiating shock drives the capsule.

Figure 2. Two designs for driving ICF capsules with Z-pinches have been fielded.

2.1 Experimental costs and constraints

Each Z shot costs about $200k split evenly between operations and projects. The operational budget covers running the machine, basic hardware, and maintenance. The projects pay for physicist time to design experiments or to analyze data, or for specialized hardware for a shot. If simulation results can provide a better understanding of the physics and reduce the need for testing by just 10 shots per year can save the program $2 million per year.

However, in reality the impact is not measured by a simple cost savings. The Z facility has limited availability of shots per year. On ZR we plan to support 250 shots per year. Typical experimental series consist of five to ten shots, allowing only 25 to 50 series each year. The true impact of modeling and simulation is to all the most useful data per shot to be collected, which in turn can allow more experimental series to be fielded.

2.2 Diagnostic data

Ten to twenty diagnostics are fielded on each shot. About 5 MB of one-dimensional waveforms are collected.

These include measurements of key parameters, such as current at various points in the machine, X-ray power, and neutron yields, all as a function of time. There is another 100 MB of image data collected. Each image can contain a large quantity of data requiring significant effort to analyze. For example, time and space resolved spectra can essentially contain 200 different measurements of the plasma density and temperature. The wealth of diagnostic data plays a critical roll in validating the computational work and developing predictive models.

3 Unresolved Science Questions

To date, advances in the Z-pinch program have occurred primarily through experiment rather than modeling and simulation. Although the Z-pinch program has made significant progress in designing radiation sources, there are several outstanding science questions that we need to understand in order to successfully design and build the next generation machine that has the goal of achieving high-yield ICF capsule ignition. We plan to use a more complete modeling and simulation capability to answer these questions.

- Wire ablation mechanisms[5] dominate the early time behavior of the Z-pinch and control the implosion dynamics, which determines the shape of the radiation pulse. Because wire ablation simulations need extreme resolution, they have been limited to single wires in 3D or a just few wires in 2D. With the high resolution ablation simulations, we have developed a wire ablation model that allows us to explore 3D system-wide effects without explicitly modeling the wires.
- The total radiated energy and radiation power are significantly influenced by the current distribution in the plasma. In Figure 1(d), plasma has stagnated on axis, but there is still trailing plasma all the way back to the original pinch radius. The exact plasma and current distribution determines the amplitude and width of the radiation pulse. There are 2D and 3D aspects to this trailing plasma.
- The experimentally observed scaling between the radiation power and the applied current for a given mass is in conflict with what is expected theoretically[4]. The scaling is somewhat less than the ideal scaling derived from zero-D analytic models. One goal of the 2D and 3D simulations is to help understand the observed scaling in order to confidently design the next generation Z facility.
- The geometry of the hohlraum containing the Z-pinch influences the implosion dynamics. The electrodes ablate plasma as the pinch is imploding. The feed gap to the electrodes is also important and causes asymmetries in the imploding pinch, which can be seen in Figure 1(d). In the future, we would like to run high resolution 3D simulations to model the walls and electrical feed, in addition to the wire array. This has already been done in reduced-resolution 2D simulations.
- In double-ended hohlraums, shown in Figure 2(a), radiation enters the secondary hohlraum through spoke-shaped electrodes rather than the solid electrodes of a dynamic hohlraum. The ablation of these spokes as the wires implode likely plays an important role in the energy coupling to the secondary hohlraum. This effect has not been explored computationally yet.
- The pinches used to support the Nuclear Survivability Campaign 7 work are, by design, not in local thermodynamic equilibrium (LTE). Non-LTE simulations require

thousands of radiation energy groups (discretization in photon energy), compared to the twenty groups typically needed for modeling a pinch near LTE. Non-LTE simulations that include limited atomic detail are only possible today in one dimension and can take weeks to run.

The complexity and size of a future predictive simulation capability depends on how many of these issues must be modeled simultaneously in one simulation. However addressing each of these items individually, as we have in the past, will certainly continue to improve our understanding of Z-pinch implosions.

For example double-ended hohlraum simulations model each phase of the experiment separately. First the pinch is imploded in 2D-RZ geometry, ignoring wall and spoke effects. This result feeds into a view-factor calculation to propagate the radiation to the secondary hohlraum, assuming the spokes and walls do not ablate. Then the capsule implosion is simulated in a separate simulation. A fully integrated simulation in 2D or eventually 3D will significantly increase our confidence in predictive simulations of this design.

4 Five year simulation requirements

In order to support the Z-pinch program, a spectrum of different types of simulations is needed. Each type has its own characteristics for size, frequency, and turn-around time. Below, are the different simulation categories as well as estimates for the resources needed in the next five years.

- Software quality practices demand that regression tests be run regularly. These tests are typically small and test a particular code feature, intending to protect the code base from unintended consequences of changes. Each developer runs the entire suite, which consists of thousands of tests, several times before each commit. The tests are also run nightly on a wide variety of platforms, including all production platforms.

  Resources: 20 runs of the suite each day * 10 processor-hours for the entire suite is a total of 200 processor-hours each day, or over 70,000 processor-hours/year.

- A more expensive suite of verification and validation problems also exists. These are run before major algorithm changes are committed and before each release. Mesh convergence studies are performed for a each problem in the suite, and some require hundreds of processors for the finest mesh resolution.

  Resources: 100,000 processor-hours to run the suite, run 10 times each year. Total of 1 million processor-hours/year.

- In the process of developing new algorithms, improving performance, or debugging user problems, developers need to run test simulations. These can range in size from a small one-processor simulation that takes seconds to a large user-simulation at the system scale. Usually, these can be reduced to a problem that runs quickly, but may require many processors. In order to make progress finding the bug or improving the algorithms, quick turn around time is needed, typically on order of an hour or so. Waiting a day or longer between development runs makes it difficult make progress on the complex issues.

  Resources: There is a range of simulations. For a team of 10 developers * 5 major tasks per developer-year * 100 simulations per task * 1-5000 processors * 1 hour to 4 days per simulation. Assuming an average of 200 processors and 3 hours per simulation, there is need for a total of 3 million processor-hours/year.

- Material models are an important input to the simulation codes. Developing an improved equation of state, conductivity, or opacity requires simulations at the atomic level to compute ensemble averages.

  Resources: 90 simulations per material * 32 processors per simulation * 96 hours * 3 materials per year is over 800,000 processor-hours/year.

- For engineering-type simulations, users need to run many simulations to explore a design space, optimize some feature, or quantify uncertainty. Since many of these simulations are needed, the fidelity of the simulations is reduced, by limiting the geometry or using coarse resolution, so that all the simulations finish in a reasonable time.

  Resources: The Z facility test shot schedule drives the simulation time to solution requirements on our computer resources. 250 Z-shots per year * 25 simulations per shot * 200 processors * 200 hours per simulation is 250 million processor-hours/year. Note that 200 processors is an average; processor counts can range from 1 to 512 or more processors, depending on available resources and actual turn-around time. This also assumes uncertainty quantification becomes routine.

- Another class of simulations explore some significant science question, and tend to be much larger and take longer. These are the capability-sized simulations that can require an entire system for an extended period of time. By more fully resolving the pinch or simulating more of the machine, these simulations can be used to develop models that improve the lower-fidelity simulations.

  Resources: 100 simulations per year * 2000-8000 processors per simulation * 500 hours is 200 million processor-hours/year. It is assumed here that we will not do uncertainty quantification on these simulations.

We expect our total need for resources to be nearly 500 million processor-hours each year, or 57000 full-time dedicated processors, or about 5 Purple-sized systems .

Our current computer usage is about 5000 full-time processors, which is about an order of magnitude less than the estimate above. With an annual growth rate in our actual usage of 60 percent over the next five years, we will reach the above estimate. Increasing the size of our current simulations, and increasing the number of simulations, which will be necessary in an environment where we rely on uncertainty quantification more, could reasonably lead to this growth rate. Moore's Law also states the growth rate in transistors on a chip grows by 60 percent annually.

4.1 Estimating data needs

A recent (and typical) simulation on Purple simulated a 90 degree wedge of a Z-pinch; each wire in the simulation was modeled with only one zone across the diameter of the wire. The 5.5 million zone simulation used 512 processors, took 250 hours (or 128,000 processor-hours), and generated 114 GB of output. The user actually restricted the data output frequency because dealing with more data is currently unmanageable; he would have preferred about ten times the output frequency. Using his ideal output frequency as a baseline, we generate about 200 kB of data per zone or 8.9 MB per processor-hour. Using the above processor-hour estimate, we will generate about 4.5 PB of data each year. Only about one-fourth of this data needs to be stored permanently.

4.2 Next-generation simulations

The estimates above are for simulations that we think we can reasonably accomplish in the next five years, given the constraints of limited system availability and limited designer availability. There are simulations in 10 to 20 year horizon that we still only dream of doing.

Given the apparent turbulent nature of Z-pinch implosions seen Figure 1, it may be necessary to fill the entire volume with a nearly uniform grid. A minimum of ten zones are needed to resolve a 10 μm diameter wire; implying that we need a 1 μm zone size. Filling the entire volume of the Z-pinch with this resolution requires about 10^{12} zones. Assuming perfect scaling from the 512 processor baseline simulation, this simulation would take 10^{10} processor-hours and generate 200 PB of data.

Admittedly, this is a rough (and large) estimation, but scaling up a current simulation to full resolution is probably the most accurate estimate possible. Given a large system, we would likely not do this particular simulation, but would rather trade resolution in the pinch for being able to model more of the system, including electrode effects (the wall or spokes), integrated transfer of the radiation to the secondary hohlraum, and even the ICF capsule itself.

5 Other needs

In addition to the computer resources needed to run the simulations, we need several other supporting technologies.

- Quantitative data analysis and reduction has always been difficult. The current set of visualization tools are good for qualitatively exploring data and understanding the physics of the simulation. The quantitative tools must be both interactive to explore large data sets scriptible to analyze the data automatically for optimization and uncertainty quantification on the compute nodes.

- Scalable debugging tools are important for improving performance and finding bugs. Debuggers, such as TotalView, should work on the same scale as the system. But lighter weight tools, such as detailed timing and memory profiling are also useful. Sometimes it is necessary to have fine-grained profiling information for each function in the code on each processor; tools to help sort through the data to find outliers are important.

- Algorithms require testing the same scale where users run, otherwise users will find the bugs and performance issues before the developers. Current system scheduling policies seem to be at odds with the code development cycle, which is much shorter than the production simulation cycle, typically hours instead of days. While it is possible to ask for dedicated time on current platforms, it might be more effective use of both system time and developers' time to have a large portion of the system permanently dedicated for development work, including both algorithm development and debugging large-scale user simulations. This would only use resources well if there are enough developers that regularly need an hour or two of compute time at scale a few times each week to keep the system utilization high. A dedicated system may be preferable to continually scheduling dedicated time for development on the one production system and interrupting critical production simulations.

- Generating a large mesh for these simulations and partitioning them so that they are load balanced is a critical first step in any simulation.

- Memory per processor must be at least held constant, if not increase. If the memory per processor decreases as the systems get larger, we will only be able to do our current problems faster and will not be able to increase resolution of the simulations or add additional physics.

6 Conclusions

The computing needs for a modeling and simulation led Z-pinch program are large and span a spectrum of computer resources. A balanced set of computer resources is needed. In particular, we estimate that we need more capacity computing resources than capability computing resources.

The estimates for the next-generation, fully resolved Z-pinch simulation are certainly daunting. Estimating future computer needs is always difficult, but five years ago if we would have thought today's 512 processor simulations impossibly large, even given access to all of ASCI Red for as long as we needed.

This is not to say that we cannot or will not make progress until we can do a fully integrated and resolved simulation. We will continue to split the problem up into manageable pieces; high resolution simulations of small features will continue to improve our understanding and to provide models enabling accurate, lower-resolution of the integrated system.

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