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ALEGRA-HEDP Validation Strategy

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ALEGRA-HEDP Validation Strategy

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Optimization and Uncertainty Estimation

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HEDP Theory and ICF Target Design

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Abstract

This report presents a initial validation strategy for specific SNL pulsed power program applications of the ALEGRA-HEDP radiation-magnetohydrodynamics computer code. The strategy is written to be (1) broadened and deepened with future evolution of particular specifications given in this version; (2) broadly applicable to computational capabilities other than ALEGRA-HEDP directed at the same pulsed power applications. The content and applicability of the document are highly constrained by the R&D thrust of the SNL pulsed power program. This means that the strategy has significant gaps, indicative of the flexibility required to respond to an ongoing experimental program that is heavily engaged in phenomena discovery.

Acknowledgements

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List of Acronyms

ASC – Advanced Simulation and Computing Program

DP – Defense Programs

DSW – Directed Stockpile Work

HEDP – High Energy Density Physics

ICF – Inertial Confinement Fusion

LEP – Lifetime Extension Program

M&S – Modeling and Simulation

MHD – Magneto-Hydrodynamics

NNSA – National Nuclear Security Administration

PIRT – Phenomena Identification and Ranking Table

R&D – Research & Development

SBSS – Science Based Stockpile Stewardship

SNL – Sandia National Laboratories

V&V – Verification and Validation

VERTS – Verification Test Suite

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Executive Summary

ALEGRA-HEDP code development and HEDP applications are coupled to a sophisticated Z-pinch experimental campaign executed by the Sandia pulsed power program. The resulting experiments are numerous (more than 200 per year) and well-diagnosed, and hence produce a wealth of data. However, from the perspective of validation of ALEGRA-HEDP for these applications, there are at least two general difficulties associated with this compendium of data:

- A great portion of the experiments are not necessarily validation-quality because of the emphasis on phenomena discovery (scientific research) and descriptive physics of wire-array Z-pinches.

- The experiments are highly integral, posing significant challenges for hierarchically planned validation projects.

It is a perverse consequence of these difficulties that the need for explanatory modeling to complement the experiments increases while our ability to validate this modeling capability also increases.

This report discusses some strategic issues resulting from the nature of the Sandia HEDP program that influence planning for validation of ALEGRA-HEDP applications. Our main conclusions are briefly summarized below:

- The Sandia HEDP experimental knowledge base tends to increase instability of the Phenomena Identification and Ranking Table (PIRT) at more detailed levels. This means that validation tasks are more reactive to recent experimental discoveries, and less in a position to drive dedicated validation experiments. While we still recommend detailed validation planning with carefully structured PIRTs, especially for Z-pinch implosion configuration applications, it must be emphasized that these PIRTs may be inaccurate in important ways.

- The PIRT in this situation is an important organizing principle for determining validation-quality data in the existing experimental database.

- Hierarchical validation is very difficult. Detailed PIRTs, even if somewhat unstable, can be helpful in unfolding hierarchical information from the integral Z-pinch experimental data.

- The critical measure of predictive confidence associated with ALEGRA-HEDP application validation is the transition from analysis of existing experiments to the predictive design of new experiments, in particular dedicated validation experiments. This transition has been accomplished for ALEGRA-HEDP application to Z-machine driven magnetic-flyer experiments.

- An important gap in ALEGRA-HEDP code verification remains the lack of dedicated verification test problems. This gap must be reduced.

1. Introduction

1.1 Approach

This report suggests a strategy for the verification and validation of the application of radiation-magnetohydrodynamics codes to SNL pulsed power program High Energy Density Physics (HEDP) research and development. This strategy is being applied to the Sandia code ALEGRA-HEDP.

The mission of the Sandia pulsed power program includes three high-level goals:

- Fundamental R&D of HEDP.
- A large-scale experimental program devoted to advancing the application of HEDP, with a significant emphasis on Z-pinch physics.
- User-facility applications of Sandia pulsed power radiation sources for NNSA programs, including specific NNSA Campaigns, such as the ICF Campaign.

Each of these goals places different specific demands upon computational modeling capability. Cross-cutting qualities of computational modeling for these goals, in any case, include *quantitatively predictive* (for design of user experiments) and *explanatory* (for theoretical work in HEDP). Quantitatively predictive modeling is essential for a high-quality experimental program, and is essential to accurately design and analyze user experiments fielded on pulsed power facilities. Explanatory modeling is essential for advancing the HEDP research program. All three of these goals are closely coupled. The cross-cutting qualities of computational modeling and the tight intersection of the broad pulsed power program mission place constraints on the verification and validation of any proposed computational modeling capability. This document elaborates this thought and suggests potential consequences.

A methodology for accomplishing verification and validation (V&V) of large-scale computational science and engineering software for predictive applications has been defined at Sandia National Laboratories under the NNSA ASC V&V program. Key references that define and explain the issues include Pilch *et al.* (2000); Trucano *et al.* (2002); Oberkampf and Trucano (2002); and Oberkampf, Trucano, and Hirsch (2004). This methodology has been systematically applied in Sandia ASC validation milestones that have been delivered or are in progress. The methodology has also influenced general planning (not directly ASC milestone related) for the application of computational modeling in stockpile Lifetime Extension Program (LEP) activities at Sandia.

The pulsed power program, while strongly correlated with the NNSA Stockpile Stewardship Program through its Campaign role, represents a significantly different challenge for application of the developed Sandia V&V methodology. This is because of the significant R&D characteristics of the program, in particular the importance of ongoing phenomena discovery experiments. While it is crucial to accomplish V&V for pulsed power HEDP computational physics modeling, it is also an interesting challenge because we expect that new elements must be added as V&V progresses because of the R&D factors. We must modify the current methodology due to (1) larger uncertainty in the implemented physics; (2) a computational physics user community that is focused more on research and less on "production;" (3) software that is highly evolutionary in response to this; (4) unusual experimental difficulties; (5) experimental efforts that have large R&D components (physics discovery). This document presents elements of a V&V strategy that will conform to the extent possible to the existing methodology, as summarized in Figure 1-1, while allowing for important uncertainties in the progress of the pulsed power program.

Figure 1-1 illustrates a schematic of the experimental validation methodology that is the central focus of ASC V&V activities at Sandia. It is important to understand the key features in this methodology.

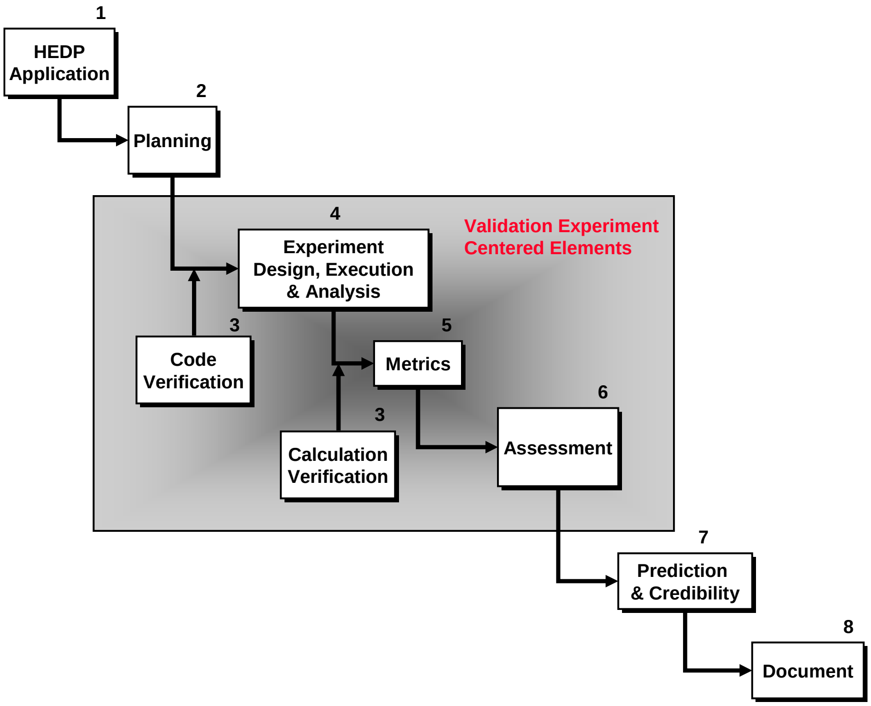

Figure 1-1. The suggested ideal validation process for pulsed power HEDP computational modeling.

1. V&V begins with the intended application of the code. In this case, the applications are to pulsed power HEDP modeling, and have major R&D factors. Applications that drive the long-term vision of the V&V strategy will be discussed further in Section 2.

2. Directed V&V is a consequence of the application requirements and needs. The strategy underlying V&V activities, presented in the contents of this document, is the recognized response to detailed understanding of these requirements and needs for the pulsed power program. Requirements and needs for the pulsed power program at Sandia are far more fluid than, for example, LEP qualification plans at Sandia. Dealing with this kind of requirements fluidity, and the future uncertainty it creates, is a challenge for this V&V effort. We suggest the development of quite high-level Phenomena Identification and Ranking Tables (PIRTs) in Section 3 as an illustration and starting point. V&V tasks related to these PIRTs should have some basic stability over the next 5 to 10 years of pulsed power HEDP research at Sandia. The validation methodology is then based on the concept that elements 3 through 8 in Figure 1-1 must respond to these PIRTs. These PIRTs are intrinsically generic given our basic uncertainty in the future technical course of the pulsed power program.

3. Verification, an assessment of the numerical adequacy of the code, centers on mathematical, algorithmic, and software implementation issues. It divides over issues that are mainly generic to the code, called *code verification* in the process Figure 1-1, and *solution* or *calculation verification*, which is specific to given calculations performed by the code. In Section 5 we will discuss these issues, specifically in the context of ALEGRA-HEDP. The code verification discussion is framed in terms of so-called *code suitability* for validation. In other words, is it reasonable to subject the code in question to validation centered on comparisons with experiments? We will explain this issue in Section 5, and discuss characterizing the suitability of ALEGRA-HEDP for the long term experimental validation activity. There are significant gaps in verification of ALEGRA-HEDP at this time.

   Calculation verification is a difficult challenge. We are asking no less than for demonstrable evidence of the *computational* accuracy of given calculations, for the particular purpose of arguing that numerical errors do not corrupt computational-experimental validation comparisons beyond the point of usefulness. In principle, we also seek rigorous proof, or substantive evidence, that calculations converge to the correct mathematical solution of the specified equations. This implies that perceived computational accuracy of given calculations, if we can measure it, is correct, and not the product of, say, mutually canceling programming or algorithmic formulation errors.

4. Elements 4 through 7 in Figure 1-1 deal explicitly with conducting experimental validation. The experimental tasks are directly linked to the PIRT, but there are major elements of uncertainty here because of characteristics of the SNL pulsed

power experimental program. To conform at least in principle to the Sandia planning and experimental validation guidance (Pilch *et al.*, 2000; Trucano, Pilch and Oberkampf, 2002) hierarchical validation experiments are presumed in this methodology. There is a suggested hierarchy of three levels of complexity that is loosely organized around (1) validation of uncoupled phenomena; (2) validation of simple couplings; (3) validation of integral couplings. In Section 5, we will discuss aspects of this hierarchy in the context of the conceptual PIRTs previously introduced. The strategy discusses the link between the anticipated experimental components and the evaluation of ALEGRA-HEDP predictive modeling capability. The R&D nature of much of the ongoing pulsed power HEDP work places a very strong constraint on our ability to make this judgment. In particular, we will be in a much stronger position to reject modeling capability than confidently extrapolate predictive capability simply because of the ongoing R&D. The simplest and most powerful measure of predictive confidence for our needs, of course, is utilization of the modeling capability to design key experiments. This process is already ongoing in one of our projected validation thrusts, that is magnetically-driven flyer plate experiments.

5. Element 8 emphasizes the belief that there is no V&V without adequate documentation. The present report is one contribution to the documentation required for V&V of ALEGRA-HEDP for pulsed power HEDP applications.

Further discussion of some items in Figure 1-1, with some emphasis on an HEDP validation strategy, is also found in Trucano (2005a).

The present document is not a frozen product, and it is only the first step of a series in developing a more complete and sophisticated validation strategy for pulsed power HEDP physics simulation at Sandia. The document develops a V&V strategy that is a snapshot in time of the needs of the pulsed power program for explanatory and predictive computational physics. Because of the R&D factors that are influencing this program as we speak, our challenge is to develop a V&V strategy that can also adapt to fundamental scientific evolution in the pulsed power program as well as decisively influence the acceptability of claims of explanatory and predictive modeling.

1.2 Constraints and Caveats

1. ALEGRA-HEDP is an R&D code, intended to support an R&D experimental program. The ultimate goal of evolution of this computational modeling capability is to guide the experimental program, not simply respond to it. This goal has been achieved for magnetic flyers, while wire arrays and z-pinch physics maturity has not been reached. This document is far less definitive than other systematic validation plans published at Sandia that are aimed at different applications, such as weapons LEP applications. ALEGRA-HEDP is currently known to be *invalid* for several intended applications; we don’t need to execute a precise plan to discover this fact. The current strategy is intended to provide a

basis for forward progress on a significantly rigorous validation strategy *as the code capability becomes more effective*.

We also assume that sophisticated users of HEDP computational capabilities are the targeted audience for this strategy and the present report.

2. The intended applications that are the focus of this specific document *emphasize MHD-governed phenomena*. For example, one key long-term need is to provide a validation strategy for assessing the validity of ALEGRA-HEDP (or other computational capability) for accurate prediction of the formation, implosion and stagnation of wire-array Z-pinches. This is only the first of two major phases in user experiments on a pulsed power facility like the Z-machine. The second major phase is typically *governed by radiation-hydrodynamics phenomena*, and centers on fielding of secondary experimental payloads that use pulsed power radiation sources. These secondary experimental packages, such as adjunct hohlraums and other interior experimental details, are driven by radiation flow and their simulation requires critical radiation-hydrodynamics phenomena. Radiation flow and radiation-hydrodynamics phenomena in user experiment configurations are not directly addressed by this initial strategy.

3. This V&V strategy is expected to rapidly evolve over at least the next two years, certainly in response to planned experimental upgrades in the Sandia pulsed power program.

4. ALEGRA-HEDP itself is the subject of significant strategic thought at the time of writing, mainly focused on evolution of new and improved M&S capabilities into calendar year 2008. The capabilities to be validated for specific applications and the intended applications in this strategy are moving targets. There is risk that even this initial definition of a validation strategy may become somewhat incoherent with the code evolution, say two years from the time of writing. It remains our hope that this document is a stable initial step in pursuing longer term V&V for application of HEDP computational capabilities.

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2. Application Definition

2.1 Definition

A key goal of modeling and simulation supporting the Sandia pulsed power program is to achieve predictive modeling that can be used for the design and understanding of complex experiments on existing facilities, as well as to credibly contribute to the design and defined application of new and more capable machines. A V&V strategy is an important step in the direction of achieving the desired high energy density physics (HEDP) modeling capability.

The purpose of computational validation efforts is to contribute to development of a physics-based understanding of present experimental performance, for example of present wire array Z-pinches, isentropic compression experiments (ICE), and magnetically-driven flyers for voltages and currents currently available. Our ultimate goal is a modeling capability that is sufficient to contribute to the current NNSA High Yield decision point scheduled to take place in FY10. Demonstrating our ability to design experiments and predict observed performance on the Refurbished Z Machine (ZR), the next improvement of the SNL pulsed power experimental capabilities, is a necessary condition for Sandia HEDP modeling to contribute to the High Yield decision point. Achieving validated initial models for ICE and flyers by the end of FY05 and wire array Z-pinches (by FY08) in principle allows our modeling capability to lead the commissioning program for ZR by confidently designing experiments for scaled ZR circuit parameters. It is important that we carefully design experiments in advance of the ZR commissioning phase to insure that we have the proper hardware and to increase our chances of meeting design goals. For the Sandia pulsed power program to prosper over the next decade (into 2014) and to maximize this program’s impact on Defense Programs in that time period, ZR must be a success. This is the fundamental driver for any pulsed power M&S validation strategy.

Figure 2-1 summarizes a strategic view of needed elements of a successful verification and validation strategy for applications of an HEDP code.

2.2 Requirements

The pulsed power program at Sandia currently intersects four NNSA weapons program Campaigns: Campaign 2 (Dynamic Materials); Campaign 4 (Secondary Certification); Campaign 7 (Nuclear Survivability); and Campaign 10 (Ignition and High Yield). The primary role of pulsed power experimental facilities for these campaigns is to develop relevant and usable x-ray sources for stockpile stewardship. To successfully perform this role requires research into the physics of fast Z-pinches (Ryutov, Derzon, and Matzen,

2000) and application of their radiative characteristics, as well as the evolution of large-scale Z-pinch facilities. Computational modeling is essential to achieve these goals. The Z Machine is a current NNSA experimental facility that provides data, through Sandia's pulsed power High Energy Density Physics (HEDP) Program, for use in directly addressing elements of these campaigns and for validating ASC codes used to provide associated modeling and simulation, as well as for dealing with issues related to Significant Finding Investigations (SFIs).

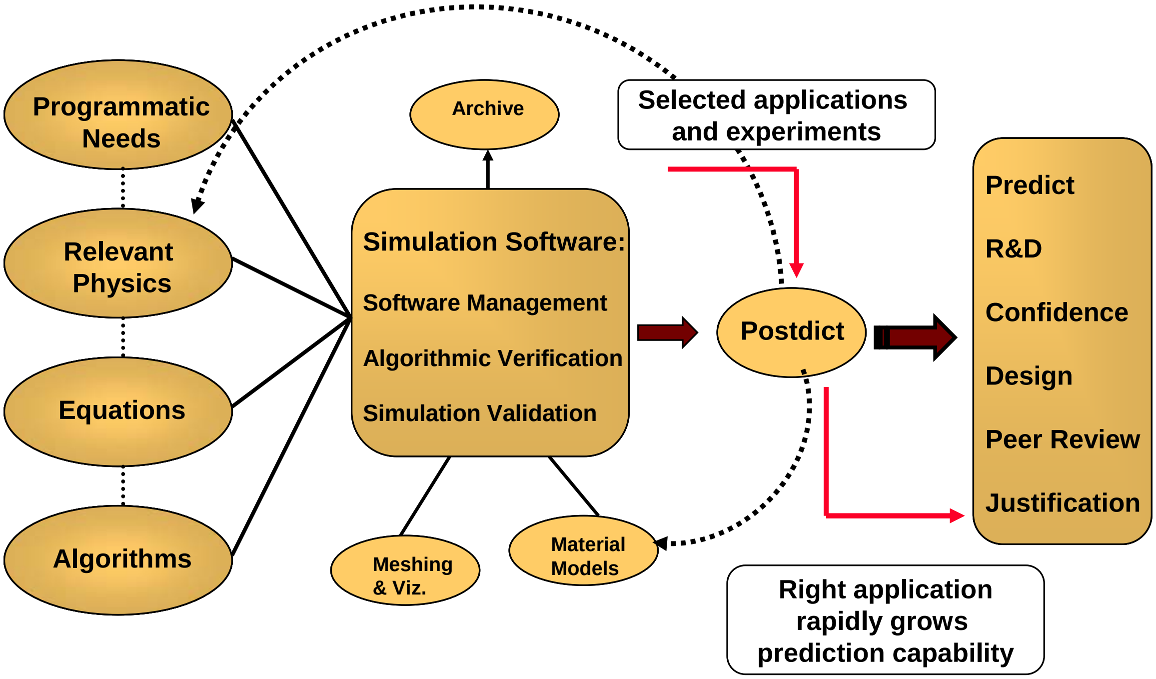

Figure 2-1. View of a successful verification and validation strategy for application of computational HEDP models.

Effective ongoing use of pulsed power experimental facilities requires a predictive design and analysis capability for guiding creation of HEDP environments and applying them to the needs of the science campaigns. ALEGRA-HEDP is the desired modeling and simulation tool that provides this capability. This ASC code solves the compressible resistive magnetohydrodynamic equations (Oliver, 2005), coupled with thermal conduction, radiation transport, two-temperature plasma physics, and an external circuit model (Carroll *et al*., 2005; Haill, Garasi and Robinson, 2004; Haill *et al*., 2005; Brunner and Mehlhorn, 2004; Haill and Cochrane, 2000). Performing these simulations depends upon a variety of complex material models, including equation-of-state (EOS), opacity and electrical and thermal conductivity models, for experimental and mission-critical materials.

In addition to the emphasis on the use of the current Z facility, the Sandia pulsed power program must also focus on future evolution of this capability. Over the next ten years, the essence of facility evolution at the heart of the pulsed power program is defined by the transition from the current Z-machine (20 MA current driven capability) to the refurbished Z-machine ZR (30 MA current) and culminating in a new facility, ZX (50 MA current). ZR is currently planned for commissioning in the FY07 time frame. In that same year, design studies for ZX must begin in FY08, targeting detailed design approval for ZX. The role of ALEGRA-HEDP predictive modeling in supporting various elements of this strategy is important.

Predictive computational modeling of HEDP phenomena that can be applied to pulsed power machine design, as well as to characterizing anticipated experimental campaigns with new facilities, is probably a necessary condition for this machine evolution, certainly for the critical decisions leading to the construction of a new machine like ZX. Modeling must contribute to design decisions as well as confident understanding of the expected strengths and weaknesses of ZR and ZX for the HEDP user community that will rely upon these facilities. An objective basis for confidence in our ability to model HEDP and the resultant radiation sources must be objectively established. To the degree that computational modeling plays a role in the believed scientific basis for future pulsed power capabilities, that modeling must have rigorously founded confidence.

The validation milestone documented in Pilch *et al.*, (2005) is the first step on the path of developing the objective basis for confidence in our understanding of the HEDP implemented in our ALEGRA-HEDP modeling tool. This milestone targets developing an initial characterization of our ability to use experimental knowledge gained from current Z-pinch operations and computational modeling of selected experiments to develop evidence of our ability to predict ZR performance with some confidence. A similar task is expected to allow us to pass from ZR experience to prediction of ZX performance in the FY07 timeframe, and should firmly build on the conduct of the current milestone. We note that Sandia also currently has an NNSA Level 1 milestone to perform the first Stockpile Stewardship experiments on ZR in FY07, and this validation milestone may have some influence on the success of this task. Modeling contributions to the design of ZX remain of critical importance.

Further discussion of underlying application requirements is given in Mehlhorn, Garasi and Trucano (2005).

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3. Phenomena Identification and Ranking Table

3.1 Introduction

The validation strategy we discuss here is compatible with the planning guidance of Pilch *et al.* (2000) and the experimental validation guidance of Trucano *et al.* (2002) to the degree that is possible subject to the caveats mentioned above. A critical element is the Phenomenology Identification and Ranking Table (PIRT), which is one means of connecting the application requirements discussed in Section 2 to actionable validation tasks.

We take a very high level view of the specification of a PIRT for this initial strategy. Deepening the important elements of the PIRT is one of the important subsequent tasks that must be performed to create a future version of this strategy. At the highest level, the PIRT for pulsed power HEDP consists of the following:

Table 3-1: General Physics PIRT for pulsed-power HEDP.

Physics	**Importance**	**Current Computational Adequacy**	**Single Phenomenon Validation Status**
Circuit			
Hydrodynamics			
MHD			
2-T physics			
Radiation			
EOS & OPACITY			
Material strength/fracture			

The high-level physics identified in Table 1 are generally described as follows:

Circuit – the physics, applied as a boundary condition, for applying stored electrical energy to MHD calculations.

Hydrodynamics – multi-material compressible hydrodynamics.

MHD - ideal, resistive MHD plus generalizations.

2T – two-temperature, single-fluid plasma physics, governing electron-ion energy partitioning and equilibration, thermal conduction, energy transport from radiation and electromagnetic conditions.

Radiation – radiation transport.

EOS & Opacity – equilibrium EOS (pressure and internal energy as functions of density and temperature); EOS transport physics (thermal conduction, electrical resistivity), opacity physics; non-LTE atomic physics.

Material strength/fracture – strength and fracture physics for solids.

We have defined three columns in this table, as follows:

Importance – this is a measure of the perceived importance of the high-level phenomenon for a defined HEDP application. A 4-point ranking scale is applied to this element:

- High: Critical for experimental comparisons.
- Medium: Sensitive factor in experimental comparison.
- Low: small effect in experimental comparison.
- None: no discernable influence on experimental comparison.

Current computational adequacy – this is a measure of perceived adequacy of current computational capabilities to simulate the stated phenomenon. This is current judgment, to be confirmed or modified through V&V tasks.

- High: No need for further improvement
- Medium: Need further improvement
- Low: Further improvement mandatory
- Unknown: assessment not performed or understood

Single physics validation status – this is a supplemental measure of the validation status of the stated physics in isolation from the other physics. This element is directed at the difficulty we face in HEDP validation that *many of the important experiments are integral,* combining most or all of the phenomena in the table. Comments in this column are intended to be descriptive.

A variety of more detailed phenomena underlie the general physics specifications suggested above. For example, if we consider Z-pinch radiation sources formed from the implosion of wire arrays on the Sandia Z-machine (Ryutov, Derzon and Matzen, 2000; Liberman, De Groot, Toor and Spielman, 1998) independent of secondary experimental configurations, several distinct phases define an underlying collection of phenomena in wire-array implosions that creates significant additional structure in any PIRT targeting an application in one or more of those phases. These phases include:

1. **Initiation** – the formation of coronal plasma, with current shunting from wire cores.

2. **Ablation** – ablation of wire cores and $\vec{J} \times \vec{B}$ acceleration of precursor plasma until local burnout of cores

3. **Foam and precursor interaction** – (related to stagnation in bare pinches and dynamic holhraums with axial foam converter structures); precursor plasma filling, foam ablation, and precursor/foam ablation interactions.

4. **Implosion** – transfer of current to wire array plasma and $\vec{J} \times \vec{B}$ acceleration of main array mass to axis.

5. **Nested array interactions** – role of nested arrays in current switching and stabilization of load implosion dynamics.

6. **Stagnation** – collision of accelerated structured load on axis (bare pinches) or on converter structure (dynamic hohlraums), shock heating, thermalization, energy equipartition.

7. **Radiation** – temporally structured radiation emission from stagnated load via bound and free electrons.

The ultimate technical requirement for a sufficient implosion configuration modeling capability is to be capable of simulating *all of these phases*.

The structure of underlying phenomenology present within these phases includes (but is not constrained to) the following:

1. **Initiation** – fluid versus kinetic plasma descriptions; physics impacts of wire impurities; origin of $m = 0$ plasma instabilities; spatial influence of cathode on initiation dynamics; characterization of and physics underlying initiation scaling phenomenology; coronal plasma dynamics and radiative characterization; relative importance of these phenomena.

2. **Ablation** – roles of Joule heating, thermal conduction and radiation; origin of $m = 0$ plasma instabilities; 3-D characteristics; characterization of and physics underlying ablation scaling phenomenology; relative importance of these phenomena.

3. **Foam and precursor interaction** – radial distribution of precursor plasma; radiative characteristics of foam converter heating and separate ablation; collisionality of foam/precursor interaction; magnetic Rayleigh-Taylor (MRT) stabilization via snowplow effect; machine top/bottom asymmetry influence; non-LTE effects in radiative phenomena; influence of foam specifications on stagnation radiative pulse shaping; relative importance of these phenomena.

4. **Implosion** – quantification of implosion deviations from ideal (0-D) behavior; influence of trailing load mass on current transfer; relative weight of MRT versus $r - \theta$ instabilities; deviation of implosion from 2-D; snowplow stabilization of MRT; machine top/bottom asymmetry influence; influence of machine electrode residual plasma; relative importance of these phenomena.

5. **Nested array interactions** – identification of optimal design parameters (mass ratios, wire numbers, initial radii); fluid versus kinetics in plasma interactions; MHD characteristics of nests (instability suppression, current switching); influence on stagnation radiation pulse shaping; relative importance of these phenomena.

6. **Stagnation** – physics of ion kinetic energy thermalization; ion-electron thermal equilibration behavior, including rates; current delivery to axis; sheath distribution and geometry (is it 3-D?); role of MHD turbulence and plasma viscosity in thermalization; influence of MHD instabilities on stagnation dynamics, structure and thermalization; relative importance of these phenomena.

7. **Radiation** – identification of dominant mechanisms for various configurations (bare pinches, dynamic hohlraums); identification of dominant mechanisms for various phases of radiation pulses (rise, FWHM, fall); termination mechanisms; disruption mechanisms; role of trailing implosion mass; relative importance of these phenomena.

Ideally, these phases and their underlying phenomena should be represented in a detailed PIRT structure underlying the high-level physics structure of Table 3-1. This is an important improvement goal for the evolution of this strategy. An example of PIRT development addressing this added detail is given by Garasi *et al.* (2005).

The most important experiments to be computationally modeled for Z-pinch related HEDP (see below) are inevitably *integral experiments* that not only combine the high-level physics we have identified in Table 3-1, but also combine the above phases and their phenomenology. It is difficult to experimentally separate the phases and detailed phenomena in a way that optimally addresses the hierarchical validation emphasized in Pilch *et al.* (2000) and Trucano *et al.* (2002). One way to characterize the consequences of this is to observe that single physics, phase or phenomena validation opportunities and results that are relevant to our most interesting HEDP applications are very desirable but *expected to be sparse*. (This is the reason that we created column three in the physics-level PIRT above.)

As explained in the general references, the PIRT is not constrained or expected to be a frozen object. This is especially true for applications with a research center-of-gravity such as HEDP applications. Execution of V&V tasks in a research context can easily create the necessity to modify the PIRT, especially our quantitative judgments about the ranked importance of phenomena and adequacy of current modeling capability for those phenomena. From the conventional perspective, identification of phenomena in the PIRT is expected to be stable. But this is precisely where the R&D emphasis of the HEDP work may have significant impact, as identification and scientific understanding of the important phenomena are evolving as a result of an active experimental research program. The subsequent V&V work must be anticipated to be more difficult because the underlying key phenomena are not a relatively stable initial condition to the work. This adds a complex nonlinearity to the planning process centered on PIRTs that makes it inevitable that PIRTs posed at any given point in the R&D process will likely change in all of their dimensions as work progresses. A V&V strategy must accept this condition as a fact of life.

3.2 Specific Example

A particular HEDP application of ALEGRA-HEDP of interest is to the analysis and design of magnetic-flyer experiments. This application and a body of ALEGRA-HEDP computational analysis is discussed in Knudson *et al.* (2001, 2003a, 2003b) and Lemke *et al.* (2003a, 2003b, 2005). This is an application in which ALEGRA-HEDP has been important, not only analyzing performed experiments but also used to design and predict optimized experiments.

A high-level physics PIRT for this application is presented in Table 3-2, with our initial input into the three columns, simply as an illustration of the kind of starting point we need for a more detailed PIRT construction.

Table 3-2. Physics PIRT for Magnetic Flyer experiment applications.

Physics	**Importance**	**Current Computational Adequacy**	**Single Phenomenon Validation Status**
Circuit	High	Unknown	Unknown
Hydrodynamics	High	Medium	Some, but informal; mainly not documented
MHD	High	Medium (Result of this validation activity)	Emphasized in this task, but not isolated.
2-T physics	Low (?)	Not relevant	Not relevant
Radiation	None	Not relevant	Not relevant
EOS - Equilibrium	High (liquid/vapor region of special importance)	Unknown	Unknown (external provider)
Material strength/fracture	None	Not relevant	Not relevant

A summary of validation work specific to this PIRT and the greater phenomenological detail underlying it is presented in Garasi *et al.* (2005). (Another document that addresses some validation issues for this application is Trucano, 2005c.)

3.3 Next Steps in Strategy

There are three distinct opportunities for validation designed around PIRTs that specialize in ways similar to the magnetic-flyer application mentioned above. These opportunities are, in order of increased complexity (more phases, more phenomena):

I. **Single wire heating and expansion.**

II. **Bare pinch implosions.**

III. **Dynamic hohlraum implosions.**

These applications involve implosion (cylindrical) hydrodynamics and significant material heating and radiation that are not tested by the magnetic-flyer application. Hence, they occupy a very important part of the application domain that is not intersected by magnetic-flyer experiments. II and III are specific cases of what we term implosion configurations. It is advantageous because it integrates fewer phenomena and can contribute to a more hierarchically structured validation effort.

As the next step in this strategy, high-level PIRTs, similar to Table 3-2, should be defined for each of these applications. Section 4 mentions an identified experimental strategy that targets bare pinches and offers an excellent opportunity to develop a detailed PIRT. This should be understood as a variation on the theme of validation for magnetic flyer applications that is discussed in Garasi *et al.* (2005). A similar strategy must also be developed for single wires and dynamic hohlraums.

Somewhat independent of the development of more specific PIRTs for these key applications, we stress two important gaps that must also be removed as part of future V&V work:

A. The ***formal hydrodynamics validation status*** of ALEGRA-HEDP has not been documented.

   There is some existing work (for example, Chen and Trucano, 2002), but was not conducted as part of a systematic hydrodynamics validation plan. An overall summary of the validity of the ALEGRA-HEDP hydrodynamics for the HEDP application domain of interest has not been developed. Such a summary requires a significant amount of new work executed to a specific hydrodynamics validation plan. This plan should be developed, either separately or as part of more detailed planning for validation of implosion configuration applications. Note that the validation that has been accomplished for magnetic-flyer applications does provide some hydrodynamics validation evidence, but this needs to be extracted from that work. Hydrodynamics is an area where significant separate physics validation can be achieved because of a variety of existing validation quality experiments.

The development of such a summary is needed and we recommend it.

B. A ***rigorous procedure for validating (or accepting) the equilibrium EOS models*** used has not been defined or implemented.

The current approach is dominated by the fact that the equilibrium EOS used in the code is third-party software and data. That is, the implemented equilibrium EOS models used in the validation tasks in this document are SESAME (LANL) and QEOS (LLNL). These are generally regarded as "community standard" models and used without detailed Sandia specific validation or acceptance testing. There are several reasons for operating in this fashion, but for really critical applications it is important to provide another level of scrutiny of these models.

The definition of a useful method for local (at Sandia) validation of equilibrium EOS models is needed but is not discussed further in this version of the validation plan. (See Trucano, 2005b for some further discussion of this issue.) Recent work on this challenge is presented in Cochrane *et al*. (2005).

This need also exists for thermal conductivities, electrical resistivities, and opacities. We suggest starting with equilibrium EOS because of greater availability of data. In any case, significant validation of these models in the warm dense matter regime independent of integral HEDP experiments will be essentially impossible. This is a problem that plagues validation of many ASC computational applications.

We emphasize these two particular gaps because they are so important for all HEDP applications with ALEGRA-HEDP. What is noteworthy about these gaps is that all applications of ALEGRA-HEDP are fundamentally constrained by the quality of work performed on these two tasks. Compressible multimaterial hydrodynamics for high-pressure high-temperature states is a necessary component of all HEDP modeling of interest to us. In turn, the quality of the multimaterial hydrodynamics that can be achieved is very strongly constrained by the quality of the EOS's used, which places another large premium on accomplishing validation of the EOS's.

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4. Validation Experiments

4.1 Introduction

The PIRT is the key link between the relevant physics and phenomena that are understood to be important and validation experiments that can be used to asses ALEGRA-HEDP capability to computationally model those phenomena. The strategy and more detailed planning must emphasize this. Here, we present a high-level view of this issue.

4.2 Use of the PIRT

The validation test matrix, that is a set of specific validation activities, should emerge naturally as an artifact of the PIRT. The ideal logical order of important relationships expressed in the V&V strategy and planning is crudely summarized as:

PIRT →

Priorities →

Needed Validation →

Responsive calculations

Validation experiments are required to close the logic. Since ASC does not fund experiments per se, there is dependence upon existing data, or new data generated by dedicated validation experiments provided by other sources, such as DP experimental activities. V&V planning should provide a strong basis for establishing data requirements, so that existing data can be assessed as to its quality for validation. Additionally, the PIRT can be used as a device to prioritize dedicated experimental work. We stress that the absence of appropriate data implies "No Validation."

The situation is less straightforward for HEDP applications. At this time, HEDP validation activities are heavily dependent upon non-dedicated experiments. This does not change the fact that some or all of the elements of experimental validation discussed in Trucano, Pilch and Oberkampf (2002) must be attended to in order to avoid vacuous validation results. Because of the research issues associated with HEDP and Z-machine utilization the ideal logic is not completely suitable for operational emphasis in our strategy.

As we emphasized in Section 3, our PIRTs are at a phenomenological level of detail hence are expected to be unstable. Primarily due to experimental phenomena discovery, but also eventually due to computational modeling insight, phenomena of importance and their ranking will change. We summarize this by emphasizing that potential validation experiments may drive the PIRT rather than vice versa as suggested by the ideal logic. By potential validation experiments we mean independently conducted experiments that achieve needed characteristics for use in validation (these characteristics are defined in Trucano, Pilch and Oberkampf, 2002). We are then likely dealing with the situation as sketched in Figure 4-1. There, we suggest that independent phenomena discovery experiments may influence the PIRT, with one (EXPT2) identified as having "validation quality," at least for the subset of PIRT physics specified.

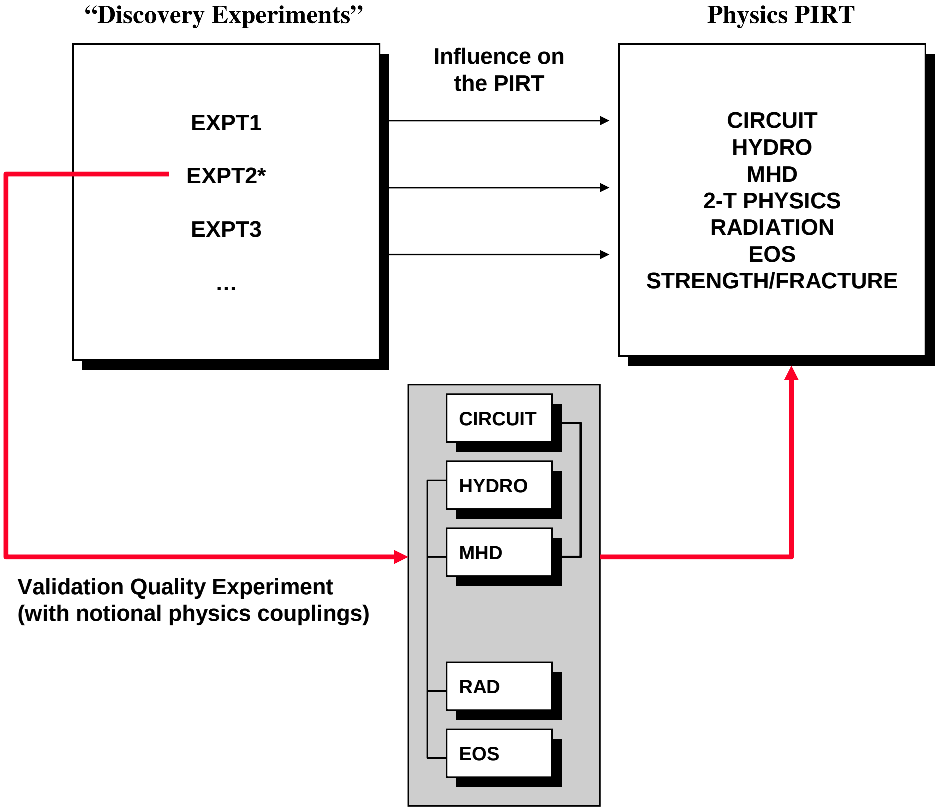

Figure 4-1. Depiction of the logic of influence of phenomena discovery experiments upon validation PIRTs (notional for ALEGRA-HEDP).

To the degree that dedicated validation experiments conforming to the guidance in Trucano *et al.* (2002) can be performed the resulting diagram of the role of the PIRT looks more conventional. See Figure 4-2.

Summarizing, for HEDP validation (and validation of research-centric code applications in general), validation must attempt to respond to both existing, independently conducted phenomena discovery experiments and to guide the performance of dedicated validation experiments. The PIRT acts as a crucial organizing principle in both cases. We also emphasize that maturation of a research code capability, for example through the execution of V&V, will be marked by a transition in time from an emphasis on independent, validation quality discovery experiments to dedicated validation experiments designed and predicted by the code. An important example of this transition for ALEGRA-HEDP is the application to optimizing magnetic-flyer experiment design (see Garasi *et al.* 2005).

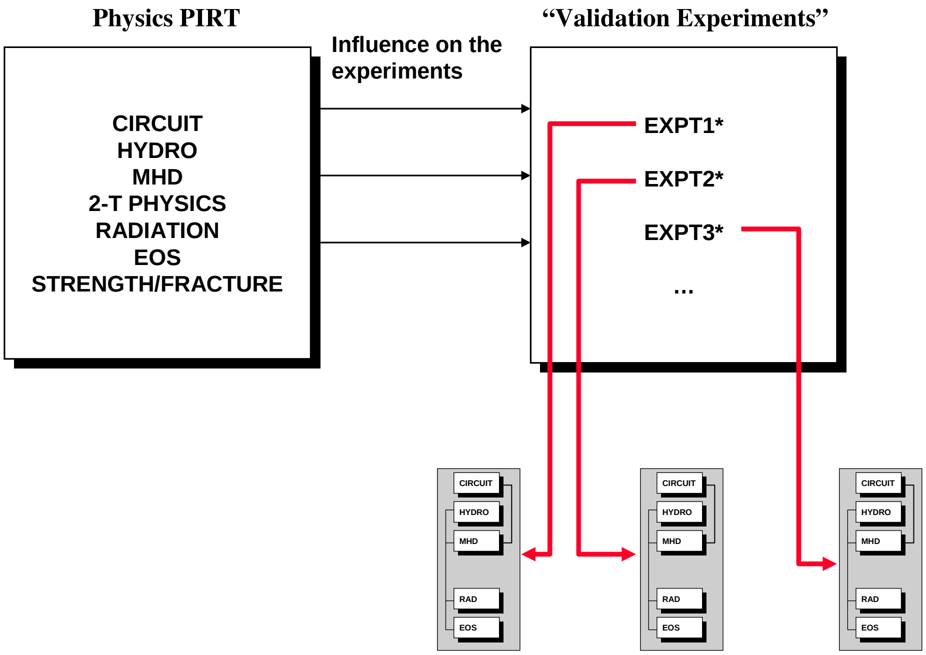

Figure 4-2. Depiction of the logic of influence of validation PIRTS on dedicated validation experiments (notional for ALEGRA-HEDP).

4.3 Experiments and Calculations

It is worth emphasizing a couple of characteristics of validation quality experiments discussed by Trucano, Pilch, and Oberkampf (2002). First, an ideal suite of validation experiments addressing a given HEDP application (for example, magnetic-flyer design optimization, wire-array implosion physics characterization, dynamic hohlraum design optimization) should be structured in a hierarchical fashion:

- Single physics (phenomenon)
- Simple coupled physics (phenomena)
- Integral physics (phenomena)

This ideal validation hierarchy is suggested by Figure 4-3.

There are many advantages to a hierarchical validation structure (see also Pilch *et al.* 2000; Oberkampf and Trucano 2002; Oberkampf, Trucano, and Hirsch 2004). But ideal hierarchical validation is unrealistic as the sole focus of validation for HEDP research applications. Typically, we are unable to achieve single physics validation experiments on relevant HEDP facilities like the Z-machine. Therefore, we are usually integrating several physics (or phenomena) in either discovery or validation experiments fielded on these facilities. For example, this is true for magnetic-flyer experiments, where high-pressure hydrodynamics, MHD, and EOS transport descriptions are integrated. This is also true for implosion configuration applications. Each of the phases for implosion configurations mentioned in Section 3 have multiple coupled phenomena, and any HEDP implosion application will integrate these phases. Thus, we are more typically facing the situation depicted in Figure 4-4, where integral experiments must be carefully understood in terms of their overlap of a hierarchically specified PIRT.

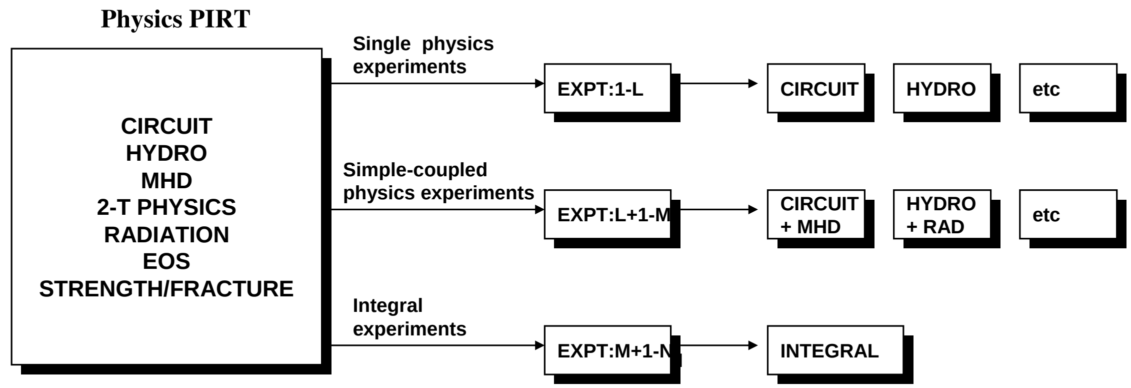

Figure 4-3. Ideal validation hierarchy suggested by PIRT (notional for ALEGRA-HEDP).

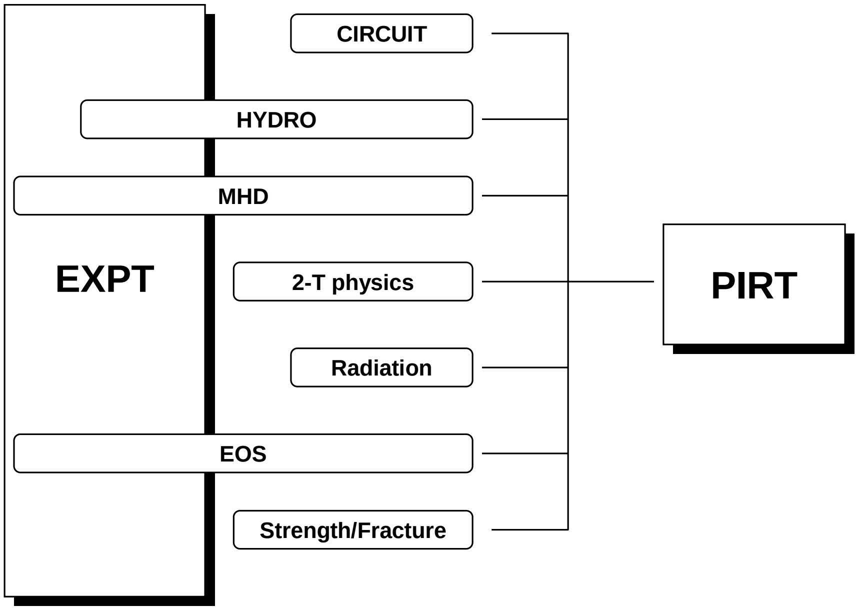

Figure 4-4. Integral experiment physics overlap with the PIRT (notional for ALEGRA-HEDP). The figure suggests that the degree of overlap of PIRT-identified phenomena is heterogeneous.

It thus is urgent to understand how high-quality integral experiments overlap the PIRT and attempt to de-convolve this information to isolate separate physics (phenomenon) validation information. This is a complex task. It can only be accomplished systematically with well-defined PIRTs. PIRT instability undermines our ability to do this to the degree that it is present.

Another crucial feature of validation quality experiments is good understanding of the uncertainty in the data. Experimental uncertainty quantification (experimental “error bars”) is another problem that is unlikely to be completely and rigorously solved for complex HEDP experiments. Some degree of experimental uncertainty quantification is a requirement for precise comparisons of experiments and calculations in validation, as emphasized in Trucano, Pilch, and Oberkampf (2002).

The components of error bars are experimental bias and variability, and various factors in real experiments enter into these components. The presentation of experimental error bars can literally be error bars on plots of experimental data. It can also be a precise discussion of what is known about that error bar. A plot that contains a calculation compared with an experiment in which no experimental “error bar” is presented or discussed invites one of two interpretations: (1) either the “error bar” is the size of the plot symbol (width of the presented experimental curve); or (2) the “error bar” is the size of the plot. In the latter case, an error bar of this magnitude implies that the calculated comparison is then meaningless.

To perform validation, even if uncertainty quantification is incomplete there must be some approximation to experimental “error bars” to provide a starting point for assessment of the experimental-computational comparisons. The minimum necessary information that should reasonably be expected for any candidate for validation data is *diagnostic resolution specifications*. Repeat experiments are, of course, of value for quantifying experimental variability. We observe that we are beginning to assert more strongly the importance of experimental repeats in our interactions with the HEDP experimental program as part of our validation strategy. HEDP experiments on the Z-machine have important variability associated with them and we will likely have to live with this for reasonable choices of data for validation usage. Recognizing this fact means that active discussion of experimental variability in our validation work is needed.

Validation calculations with ALEGRA-HEDP are subject to equivalent needs. Validation calculations are the calculations that are compared with experimental data for the purpose of inferring physical quality (physical accuracy) of the calculations for the application represented by the chosen validation data. Comparisons of calculations and experiments for validation require a precise understanding of the presented comparison, which is typically in the form of plots, but could also be detailed tabular comparisons or other quantitative representations of the comparison. This means that, in addition to the uncertainty in the experimental data, the numerical accuracy of the presented calculation(s) must be acknowledged and accounted for in the details of the comparison. The fundamental question that must be recognized, if not completely answered, is “Does the numerical error fatally corrupt the comparison with experimental data?” In the absence of acknowledgment of this problem, comparison with experimental data is irrelevant.

Solution verification is another term for quantification of the numerical error in a presented calculation. This is all but impossible to perform completely and rigorously for complex calculations. (And this raises the level of importance of Verification Test Suites and of numerical sensitivity studies. This is further discussed in Section 5.) However, it can be partially and practically addressed by mesh robustness and convergence studies, formal error estimation procedures, and inference from test problem suites. Past computational experience can also count for much if properly understood and presented.

A common fallacy is to effectively ignore the problem, observe good agreement with experimental data by means of the chosen comparison, and then conclude that numerical accuracy is good. Numerical accuracy is not measured by comparison of calculations with experimental data. One simple counter example is the presence of mutually canceling bugs in a code that happen to lead to fortuitous agreement with selected data. Another example is to observe agreement with experimental data at one mesh resolution, and then see the agreement worsen as the mesh is resolved. If mesh refinement studies are not performed this problem will never be observed.

Ideally, beyond solution verification uncertainty quantification of calculations should also be performed, mirroring the need for this on the experimental side. Uncertainty in calculations is different than solution verification, although not knowing numerical error in a given calculation is also an uncertainty (a lack-of-knowledge uncertainty). Rather, validation calculation uncertainty quantification addresses the presence of true uncertainty (variability or lack of knowledge) in parameters (for example experimental parameters) that govern the calculation. Examples include natural variability in a needed parameter (a classic example is the choice of seeding for random perturbations that are used in wire array implosion studies) and lack of knowledge about parameters (such as the "correct" value for a crucial equation of state parameter). Calculation uncertainty quantification also reflects uncertainty in the experimental data needed to define appropriate validation calculations, for example initial and boundary data.

Calculation uncertainty should at least be acknowledged in the comparison of calculations with experimental data. This can be accomplished through classical computational physics sensitivity analyses. Or it can be addressed with systematic uncertainty quantification (UQ) procedures, for example through the use of the DAKOTA UQ toolkit (Eldred *et al*. 2001). Of course, there are currently constraints on our ability to compute large ensembles of complex calculations to achieve some measure of uncertainty quantification on even the most capable ASC computers. To the degree that a computational-experimental comparison has some quantified uncertainty, however, validation inference about the meaning of the comparison should factor in that knowledge.

For magnetic-flyer applications, we have been able to utilize validation quality experimental data and calculations with some quantification of accuracy and uncertainty, yielding significant validation conclusions (Garasi *et al.* 2005; and Trucano 2005c for some additional commentary). For implosion configurations, we are only in the initial phase of this strategy. Our current emphasis is to simply understand the important existing experiments and their role in PIRT-structured validation. For example, Cuneo (2005a, 2005b) has provided an important documented aggregation of existing bare pinch implosion experiments on the Z-machine for use in validation of ALEGRA-HEDP for implosion configuration applications. Some analysis of this material and its influence on development of a detailed PIRT for implosion configuration applications is also found in Garasi *et al.* (2005).

4.4 Next Steps

A short-term emphasis has to be understanding and organizing existing experimental data into a rigorous validation structure for implosion configurations. As part of this effort, we must also recognize that our current ability to design and predict dedicated validation experiments is dependent on an evolving code capability with ALEGRA-HEDP that is itself a research program. Our ultimate success is measured by how successful this transition is.

Detailed summaries of existing potential validation quality experiments should be developed for each of the three wire-array related applications mentioned in Section 3.3. The work of Cuneo and subsequent analysis of this information essentially accomplishes this task for bare implosions. A similar process should be executed for single wires and dynamic hohlraum implosions.

An important element in the information developed by Cuneo was a discussion of data quality (Cuneo, 2005b). This is necessary for any appraisal of validation quality of these experiments, and thus needs to be replicated for single wires and dynamic hohlraums.

The transition of capability to credibly design implosion experiments should be marked by a re-evaluation of the underlying PIRTs, with recognition of the transition from validation activities driven as described in Figure 4-1 to those driven as in Figure 4-2. The successful magnetic-flyer application validation of ALEGRA-HEDP is a paradigm for the forward strategy for implosion configuration validation.

5. Verification

5.1 Introduction

Verification has two distinct components that support validation work, code verification and solution (or calculation) verification.

Code verification is the accumulation of evidence that the mathematics, solution algorithms, and software implementation in ALEGRA-HEDP are correct. Some evidence of code verification is a necessary condition for belief that the code should be used in validation, as well as application, calculations. Definitive solution of an open-ended problem like code verification is not possible. But validation depends on the degree to which we have accumulated enough evidence to justify performing validation calculations. This is the primary goal of code verification from the perspective of our strategy.

The ALEGRA-HEDP ASC Level 2 validation milestone statement (Pilch *et al.* 2005) expresses the need for code suitability assessment for pursuing validation. Code verification evidence is included in such an assessment through three primary elements:

- Existence of evidence that ALEGRA-HEDP is released and maintained to Sandia ASC software quality engineering (SQE) guidance (Boucheron *et al.* 2005a, 2005b).

  All ASC codes at Sandia are required to conform to the published guidance and have evidence to this effect. As an ASC code ALEGRA-HEDP is in conformance with this element. (This is discussed in greater detail in Garasi *et al.* 2005).

- Development of an ALEGRA-HEDP issue and bug log, and correlation of this log with proposed validation calculations (our current emphasis).

  The rationale here is that code capabilities with known bugs or performance-destroying issues can’t be relied upon. ALEGRA-HEDP maintains a current issue/bug log that is accessible to its user community as well as the developers. (This is discussed in greater detail in Garasi *et al.* 2005.)

- Existence of ALEGRA-HEDP verification evidence centered on specification and execution of verification test suites (VERTS) with problems relevant to proposed validation calculations.

  This element is of particular concern to us in this report, because a forward validation strategy must address recognized gaps in ALEGRA-HEDP VERTS relevant to HEDP validation and application calculations. We discuss this strategic issue below.

- Evidence of relevant ALEGRA-HEDP documentation for theory, algorithms and software.

  Code verification can be achieved to a very high degree and one could still question the usability of a code. Usability rests on the release and maintenance element of SQE, but also on useful documentation. Significant ALEGRA-HEDP documentation exists (see the references in this report), but there are also significant gaps. Garasi *et al.* (2005) provide discussion of the expected user community for ALEGRA-HEDP (research oriented) and current project activities addressing documentation issues.

Solution verification was defined in Section 4. Solution verification is critically important, but in two respects more detailed discussion is beyond the scope of this report. First, real steps to understand solution verification are quite dependent on the specific calculations undertaken. Therefore, detailed discussion is properly in the context of a specific calculation. Garasi *et al.* (2005) present solution verification information about specific magnetic-flyer validation calculations.

Additionally, in principle solution verification is also broadly addressed by computational technology, especially a posteriori error estimation (Oberkampf and Trucano, 2002; Oberkampf, Trucano, and Hirsch, 2004). Such technology does not currently exist for ALEGRA-HEDP and its development is yet another research problem and well beyond the scope of this report. Attention to improving error estimation technology for ALEGRA-HEDP is certainly an important long-term strategic issue, however.

5.2 Verification Test Suites for ALEGRA-HEDP

Verification test suites (VERTS) are strategically linked to the PIRT and validation tasks spawned by it. A broad discussion of this linkage is given in the fundamental planning document of Pilch *et al.* (2000). In that document a single VERTS is defined, having a structure that ideally reflects the validation hierarchy (single phenomenon, simple coupled phenomena, integral). Here, we prefer to advocate a VERTS strategy that consists of multiple suites of test problems. This helps us link strategic VERTS development to the physics structure we discussed in Section 3, as well as acknowledges the difficulty of expertly maintaining a single large, complex verification test problem suite.

A *verification test problem* is a strong test of the code. That is, the correct answer to the test problem is known and is used to assess code performance on the test problem. While solution verification is also important when executing verification tests, the tests themselves are aimed at code verification. The assessment enabled by verification test problems assesses the correctness of mathematics, algorithms, and software. This does not mean that failure of the code on a specific VERTS test problem is necessarily easily traced to some specific math, algorithm or software. Anybody who has tested a code like ALEGRA-HEDP knows how difficult it can be to pin down the specific source of failure on a test problem. But the logic of using such test problems is precise. Failure of ALEGRA-HEDP on a VERTS test results in a rigorous determination that something is wrong and must be fixed. If the VERTS test is related to a validation problem or application of interest, then this failure unambiguously cautions the alert user against that particular use of the code.

As emphasized in Pilch *et al.* (2000) a VERTS must be specified in three critical dimensions:

- Relevance – why is the stated test problem of use or importance?
- Specification – all details of problem definition must be presented. Reproducibility and traceability are the goals.
- Assessment – the principles and methodology underlying assessment must be specified. In particular, the definition of pass/fail for the test must be provided. (This is not necessarily easy.)

For example, VERTS tests can be sanity checks (conservation of energy; preservation of symmetry); problems with analytic or quasi-analytic solutions (closed-form solutions of subsets of rad-MHD equations for ALEGRA-HEDP, for example); or problems with approximate solutions having a high degree of credibility (numerical solutions of similarity equations for the hydrodynamic equations in ALEGRA-HEDP, for example). Other code calculations may also be suggested as VERTS tests. However, we point out that the use of code comparisons as a verification test (or a validation test) has been strongly discouraged by the Sandia ASC V&V program (Trucano, Pilch and Oberkampf, 2003).

In this report we do not discuss specifics of either specification or assessment of ALEGRA-HEDP VERTS, as this goes well beyond our purpose. The dimension of relevance is worth some discussion, however, because the PIRT (both at a high level and a more detailed level) provides an excellent mechanism for establishing problem relevance.

Validation requires that the code that implements the phenomena that are detailed in the PIRTs must be subjected to verification scrutiny. This implies that a verification test problem’s relevance can be automatically established by showing its relevance to the PIRT. This can be directly accomplished by directly linking to the test to the phenomena identified in the PIRT, that is:

PIRT Phenomenon P → verification test suite.

For example, for the high-level physics PIRT discussed in Section 3, we recommend that a series of VERTS be established, along the lines of:

Circuit Equation → Verification test suite

Hydrodynamics → Verification test suite

MHD → Verification test suite

2-T physics → Verification test suite

Radiation → Verification test suite

EOS → Verification test suite

Opacity → Verification test suite

Material strength/fracture → Verification test suite

This represents single physics VERTS development. We also need coupled-physics VERTS defined. Important cases for HEDP applications include:

Rad-Hydro

Rad-Hydro-2T

Rad-MHD

Rad-MHD-2T

Developing tests with this degree of phenomena coverage is difficult. But, verification test problems exist or can be constructed for essentially all of these elements. (Needless to say, having a VERTS with a couple of sanity checks and one good semi-analytic solution is better than having no VERTS at all.) The larger issue is putting all of these test problems together in a meaningful and manageable way, including the procedures required for high-quality assessment of code performance on them. This includes methods for systematically and repeatedly executing the tests. This requires a well-designed and implemented test infrastructure that currently does not exist for ALEGRA-HEDP.

An example of initial steps in verification testing of ALEGRA-HEDP is given by Brunner, Rochau and Kurecka (2004).

5.3 Next Steps

We cannot underestimate the importance of developing appropriate sets of VERTS, correlated with the PIRT structure, for validation of ALEGRA-HEDP applications such as magnetic-flyers and implosion configuration simulation. The tests embodied in the defined VERTS must be cyclically applied within a rigorous test framework, with careful accumulation of precise assessments. To even approximate success in this endeavor therefore requires two major contributions:

- Significant subject matter expertise focused on the development and accumulation of appropriate VERTS test problems.
- Construction and implementation of a test infrastructure that optimizes the human effort involved in verification testing as well as the code verification impact of cyclically executing these tests.

The forward strategy must be to address both of these contributions. Initial steps are described in Garasi *et al.* (2005). We believe that a VERTS strategy encompassing both of these factors should be conceived and documented. This is a problem for the Sandia ASC V&V program as a whole. Some preliminary thinking on this topic has been performed by Knupp (2005); further integral program guidance on this matter is expected in the future. The developed ALEGRA-HEDP VERTS strategy should carefully intersect this program guidance, and may have some influence on its development.

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6. Conclusions

The primary applications of ALEGRA-HEDP at this time are to support an exploratory research, development, and application HEDP research program at Sandia. Current experiments, often phenomena discovery experiments, are driving this program. There are two main phases, somewhat temporally serial, for ALEGRA-HEDP to deliver major impact on this program:

I. Analysis – use of ALEGRA-HEDP to analyze and understand existing experiments.

II. Prediction – use of ALEGRA-HEDP to design and predict experiments.

The transition from experimental analysis to confident experimental design and prediction of to-be-performed experiments is the fundamental measure of predictive confidence that this validation strategy is based upon. The transition to predictive experimental design is almost inevitable if we can successfully achieve validation of the current key applications for implosion configurations. We have successfully achieved this transition for the case of magnetic-flyer applications, which therefore serves as an important paradigm for our hopes and expectations of validation of implosion configuration applications.

ALEGRA-HEDP is itself a research code, with many known current limitations, issues, and bugs. Reduction of these limitations, issues and bugs is to a greater or lesser extent part of the research content of the HEDP program.

Because of the research environment in which ALEGRA-HEDP is developed and applied, V&V is a challenge. In particular, a key device for achieving rigorous validation, the PIRT, sits on tenuous ground. Phenomena are being discovered, explored, ranked in importance as a function of time, and this makes the PIRT a variable entity. The ultimate threat is that new experimental discoveries could completely upend the PIRT. The variable nature of PIRTs was recognized by Trucano, Pilch and Oberkampf (2002), but this variability is potentially much greater for a research-focused code like ALEGRA-HEDP.

This suggests that a separately developed and documented high-level strategy for HEDP application validation of ALEGRA-HEDP is useful and may help enable more detailed validation planning and execution.

We conclude with the following observations:

- The Sandia HEDP experimental knowledge base tends to increase instability of the Phenomena Identification and Ranking Table (PIRT) at more detailed levels. This means that validation tasks are more reactive to recent experimental discoveries, and less in a position to drive dedicated validation experiments.

While we still recommend detailed validation planning with carefully structured PIRTs, especially for Z-pinch implosion configuration applications, it must be emphasized that these PIRTs may be inaccurate in important ways.

- The PIRT in this situation is an important organizing principle for determining validation-quality data in the existing experimental database.

- Hierarchical validation is very difficult. Detailed PIRTs, even if somewhat unstable, can be helpful in unfolding hierarchical information from the integral Z-pinch experimental data.

- The critical measure of predictive confidence associated with ALEGRA-HEDP application validation is the transition from analysis of existing experiments to the predictive design of new experiments, in particular dedicated validation experiments. This transition has been accomplished for ALEGRA-HEDP application to Z-machine driven magnetic-flyer experiments.

- An important gap in ALEGRA-HEDP code verification remains the lack of dedicated verification test problems. This gap must be reduced.

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