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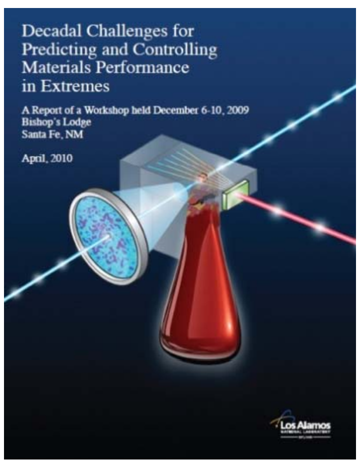
Title:	MaRIE: An experimental facility concept revolutionizing materials in extremes
Author(s):	Sarrao, John L.
Intended for:	Briefing for Sen. Heinrich staff

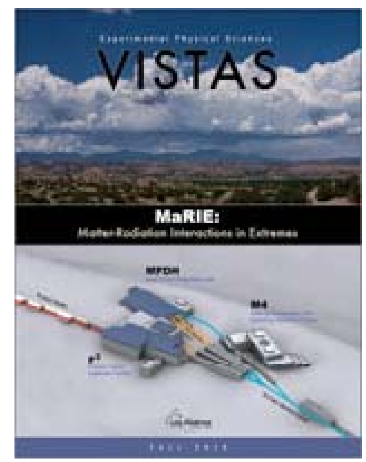
MaRIE:

(**Ma**tter-**R**adiation **I**nteractions in **E**xtremes)

An Experimental Facility Concept Revolutionizing Materials in Extremes



John Sarrao
Los Alamos National Laboratory



Sen. Heinrich Visit
02/01/13

A brief history of MaRIE

(2006-2008)

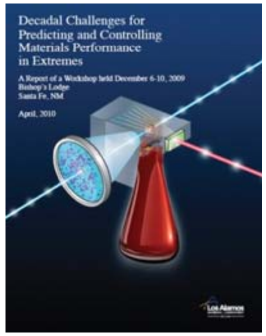
LANS Contract Transition

Concept Definition/Internal Competition

MaRIE selection

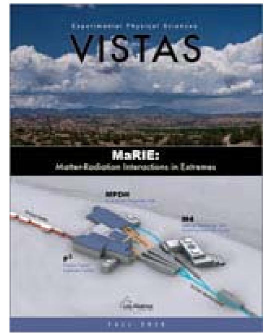
Pre-MaRIE

Science Need



(2009)

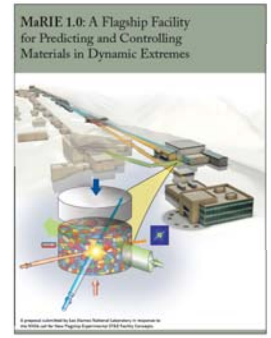
Facility Definition



(2010)

MaRIE 1.0

Pre-conceptual Proposal



(2012)

Near Term (FY12) – "MaRIE Proposal":

MaRIE 1.0: Response to NNSA "New Facilities" Call and Path to CD-0

Medium Term (FY12 → FY15) – "MaRIE Project":

Facility-specific risk reduction r&d with partners (e.g., SLAC)

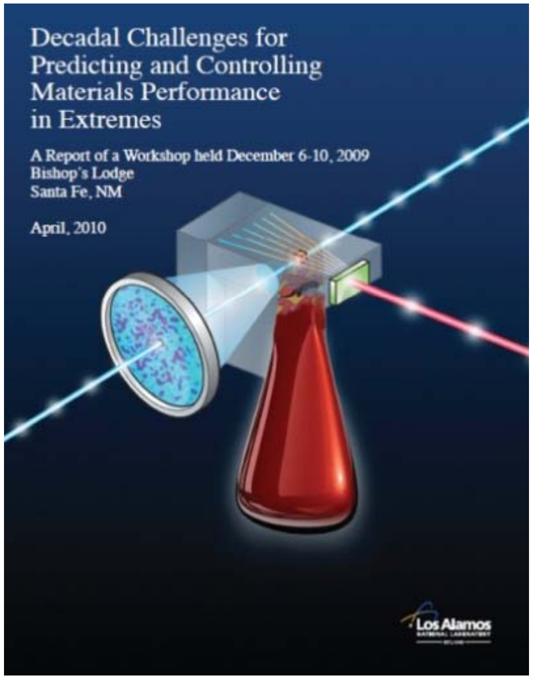
Ongoing –"MaRIE Program":

Institutional investments (e.g., related LDRD): Materials in Extremes, Co-Design, …)

External collaborations: CMIME (BES), CASL (NE), ExMatEx (ASCR)

Materials research is on the brink of a new era – from observation of performance to control of properties

The confluence of unprecedented experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

in extreme environments

dynamic loading, irradiation

coupled with predictive modeling and simulation

materials design & discovery

MaRIE builds on the LANSCE facility to provide unique experimental tools to meet this need

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

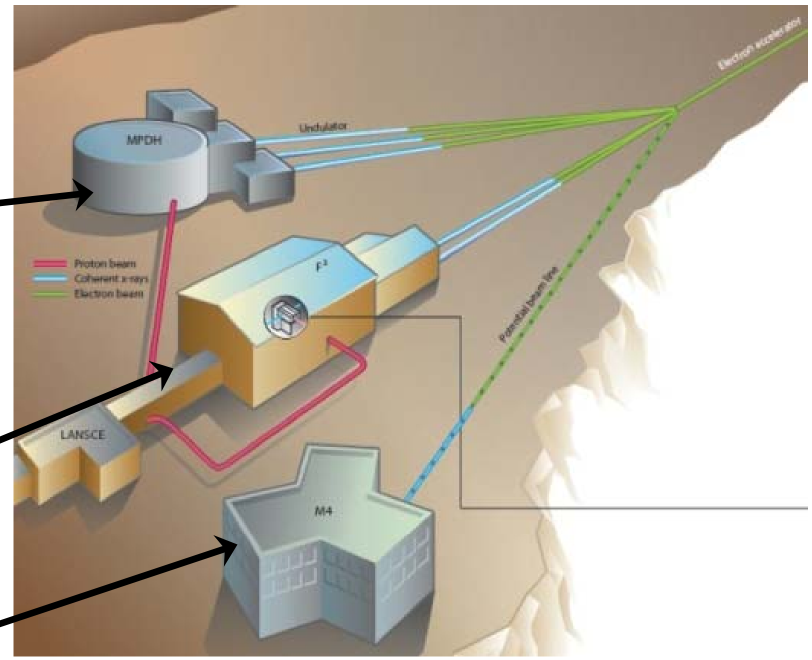
(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

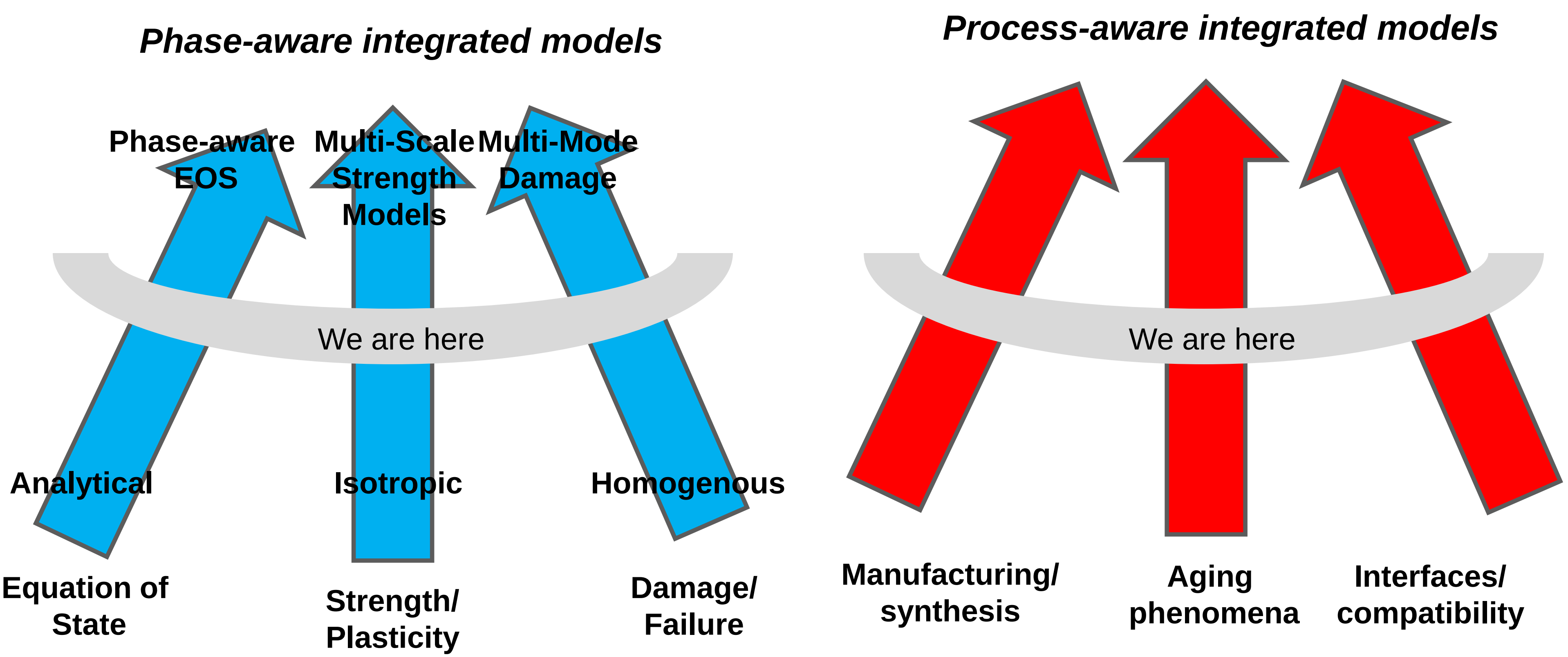
(**M4**: Making, Measuring & Modeling Materials Facility)



Unique very hard x-ray XFEL
Unique simultaneous photon-proton imaging measurements
Unique spallation neutron-based irradiation capability
Unique in-situ, transient radiation damage measurements
Unique materials design and discovery capability

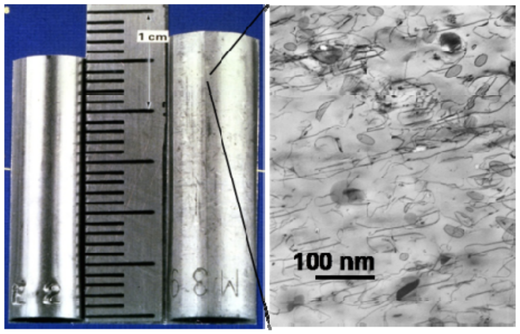
MaRIE will provide unprecedented international user resources

(In the weapons program,) we have not yet achieved a predictive, process-aware understanding of materials performance



An integrated suite of fundamental, focused, and integrated experiments is required for success

Materials behavior limits the performance of advanced energy systems needed for energy independence

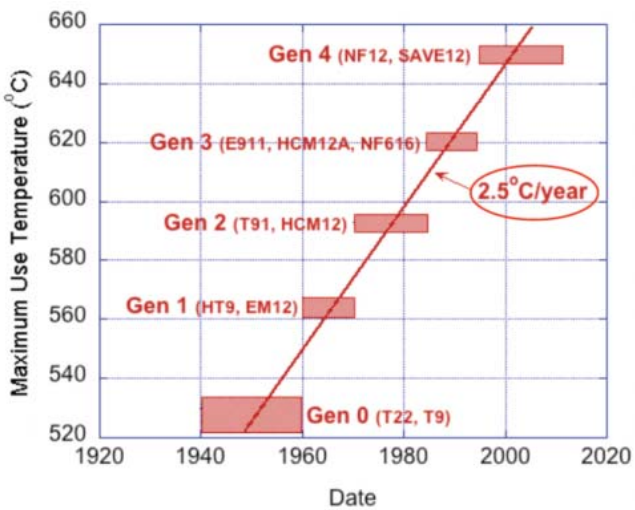


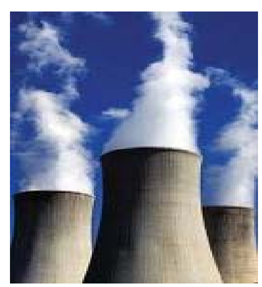
Life extension, safety of existing reactor fleet

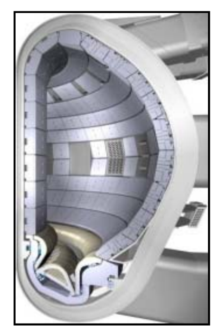
Improved affordability for new reactors

Sustainable fuel cycles

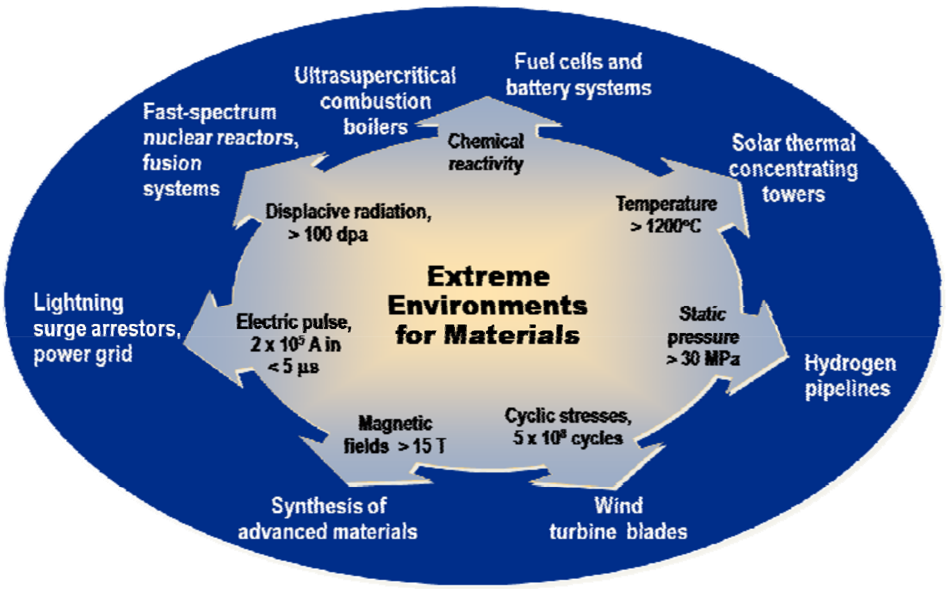
Fusion Reactor first wall materials

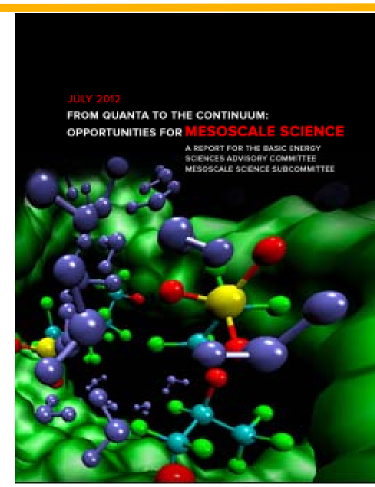


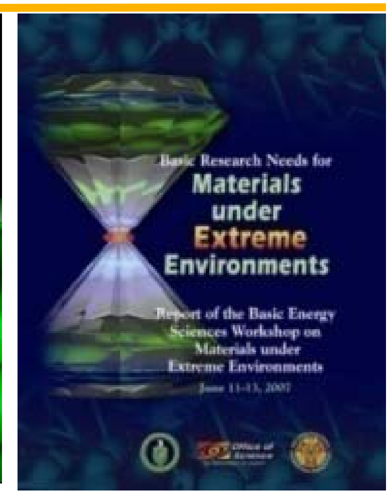




The needs for materials in extremes are many; the challenge is common: revolutionary advances in controlled functionality



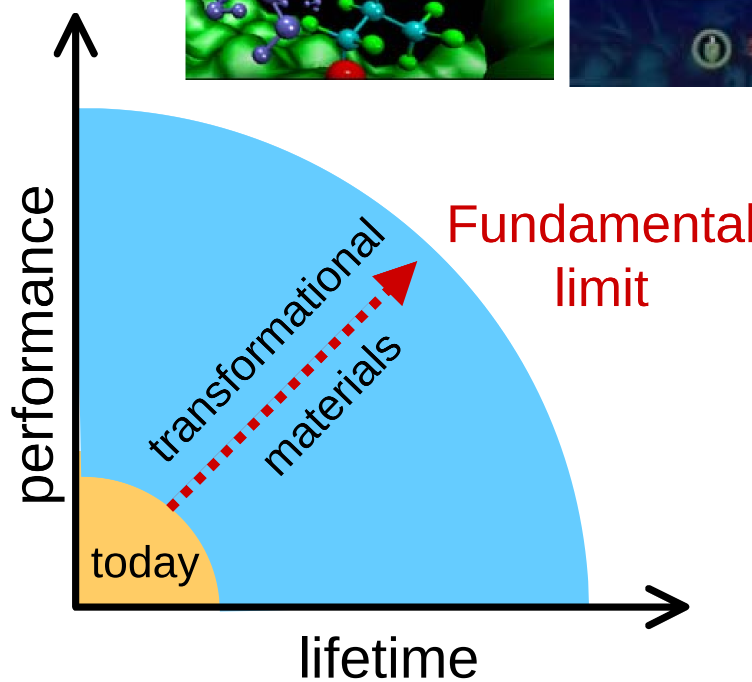




We need to enable a transition:

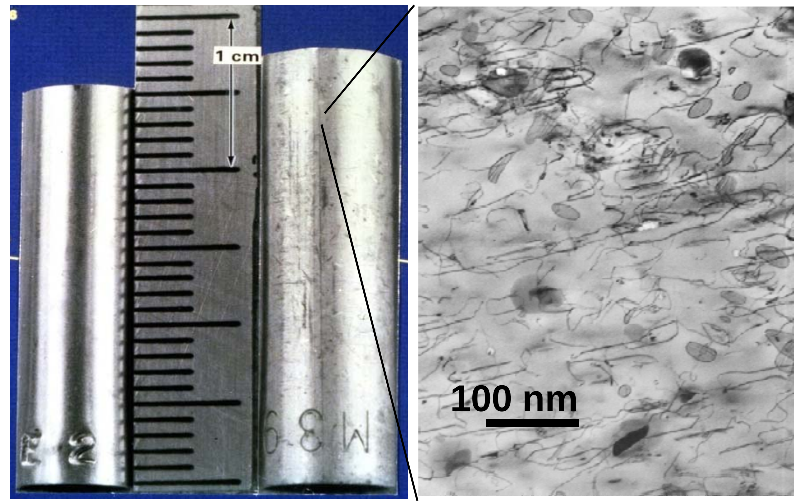
from observation and validation

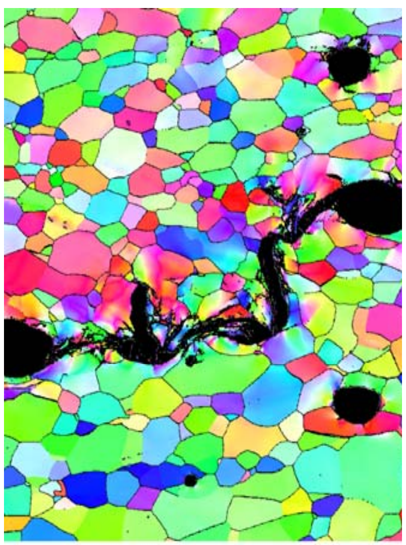
to prediction and control



The "micron frontier:" Bridging the gap between atomic understanding and bulk performance

~ 1 μm is the domain of defect consequences and microstructure interactions that drive materials strength, damage evolution, etc.

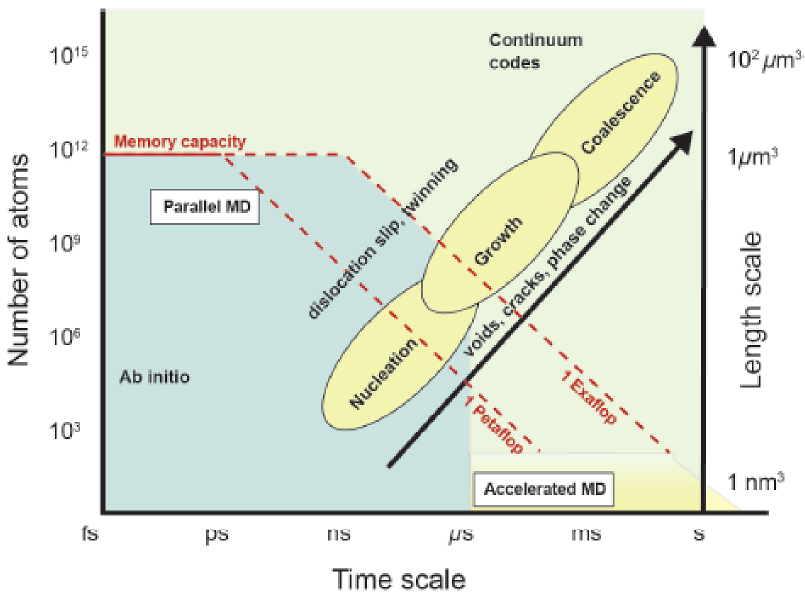




100.0 µm = 100 steps Boundary levels: 15° IPF [010]

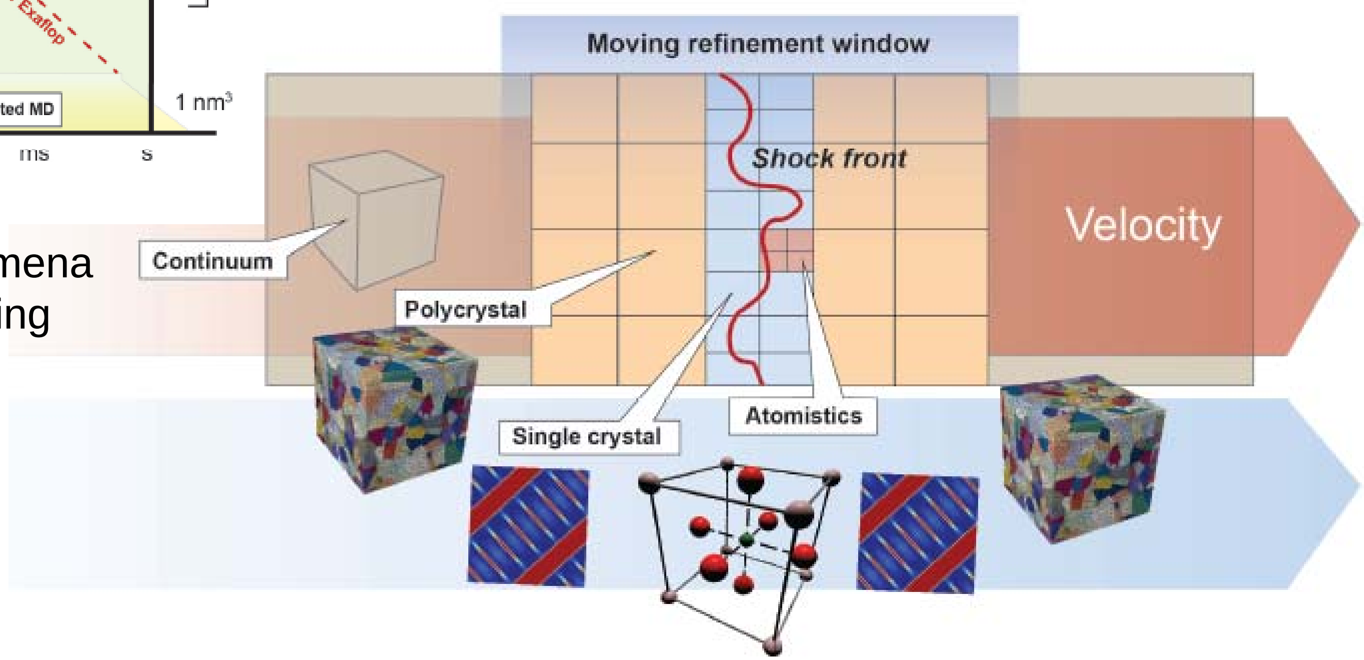
Dynamic, stochastic processes in extreme environments dominate the phenomena that we do not understand

MaRIE will yield an innovative coupling of multi-scale theory and multi-probe experiment on next-generation computing architectures

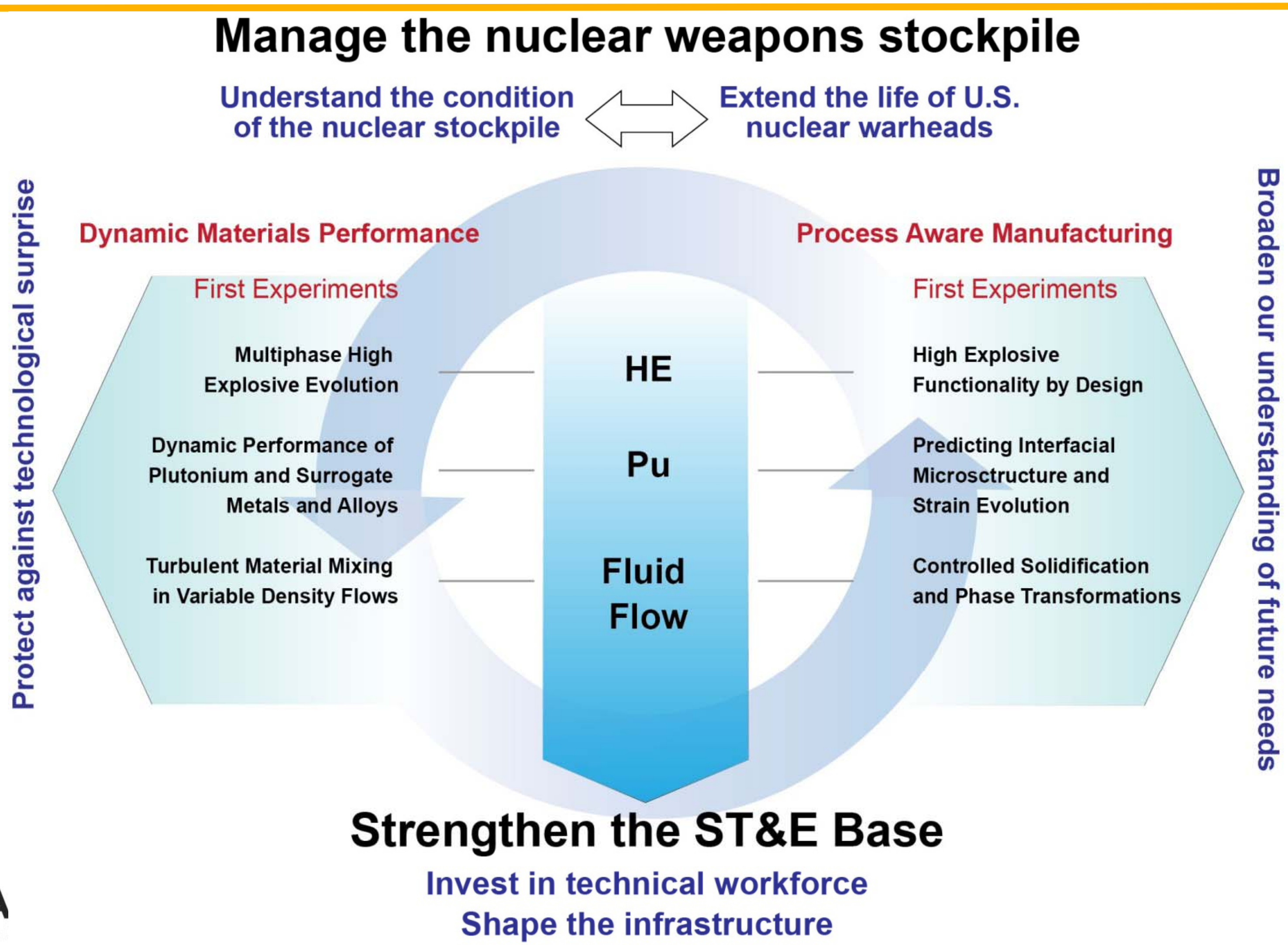


Mesoscale materials phenomena need extreme-scale computing

Variable-resolution models are synergistic with multi-probe in-situ, transient measurements



A family of MaRIE 1.0 “First Experiments” span the mission need AND set functional requirements for the facility



MaRIE 1.0 “First Experiments” define mission-driven functional requirements and reveal performance gaps

Mission Need | **First Experiments** | **Functional Requirements** | **Performance Gaps**

First Experiments

Dynamic Materials Performance
- Multiphase High Explosive Evolution
- Dynamic Performance of Plutonium and Surrogate Metals and Alloys
- Turbulent Material Mixing in Variable Density Flows

Process Aware Manufacturing
- Controlled Solidification and Phase Transformations
- Predicting Interfacial Microstructure and Strain Evolution
- High Explosive Functionality by Design

Functional Requirements

Environments
- Dynamic pressure: 4–200 GPa
- Strain rate: 10^{3}–10^{7} s^{-1}
- Stress loading > 200 ns
- HE < 500g (< 30g with SNM)
- Temperature rate 10^{5} °C/sec

Transient Multi-frame Measurements

Imaging
- 0.1–1 µm, < 0.3 ns res over 0.1–1 mm
- 0.1–1 nm, < 1 µs res over 10 µm
- 1% density accuracy

Diffraction
- Defects: 1 nm res over 10 µm
- Phase: 1–2 µm res over 100 µm
- Lattice Strain: 10^{-5}–10^{-3} over 10’s of µm

Thermo-Physical
- Temperature: 10 µm and 10–100 ns res
- Chemistry 1 µm; < 100 fs

Synthesis with *in situ* Characterization
- Single crystals and 2D interfaces
- Tailored microstructures with control of grain size, phase, and composition
- HE and actinides, metal alloys
- Real-time feedback during processing

Performance Gaps

Integrated Driver Suite

Repetitive 42-keV coherent x-ray source with 10^{10} photons in < 1ps focused to 1–100 mm

Dynamic charged particle imaging with 12-GeV electrons and 0.8-GeV protons

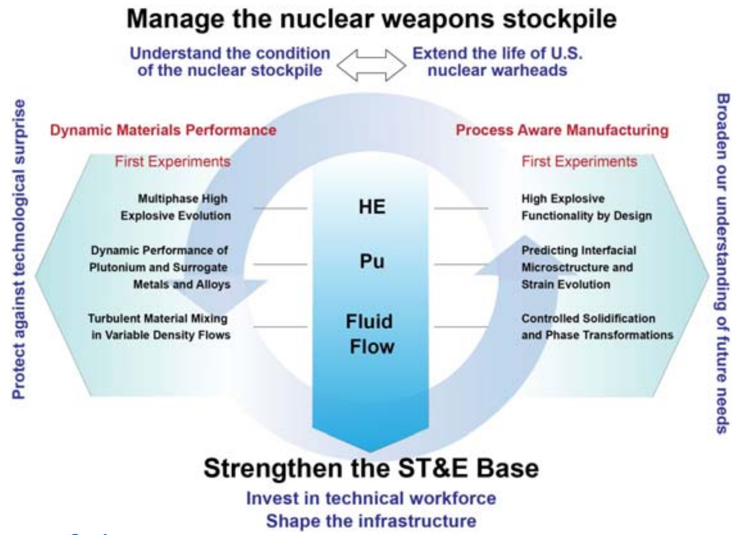
Synthesis, characterization, and processing with control of impurities and defects

Integrated co-design and data visualization

"First Campaigns" illustrate the business case for MaRIE 1.0: predict and control → certification and qualification

"First Experiments" span mission need and set requirements

"First Campaigns" span a set of "First Experiments" (and other work) to meet milestones and are **examples of how MaRIE 1.0 would help address today's problems**



"Needed science to support LEPs" (Bernardin)

1. Design and prove-out of conceptual designs for future applications
2. Advancement of certification strategies
3. For reuse-based concepts, determination of which components can be reused, which can be satisfactorily remanufactured, and for those that need replacement, appropriate replacement materials
4. Maturation of weapons components

Controlling mesoscale materials properties directly impacts LEPs

LANL (and SNL & LLNL) are actively working responses to the NNSA New Facilities Call

NNSA

Department of Energy
National Nuclear Security Administration
Washington, DC 20585

SEP 16 2011

MEMORANDUM FOR PAUL HOMMERT
PRESIDENT AND LABORATORIES DIRECTOR
SANDIA NATIONAL LABORATORIES

CHARLES MCMILLAN
DIRECTOR, LOS ALAMOS NATIONAL LABORATORY

GEORGE MILLER
DIRECTOR, LAWRENCE LIVERMORE NATIONAL LABORATORY

FROM: DONALD L. COOK
DEPUTY ADMINISTRATOR
FOR DEFENSE PROGRAMS

SUBJECT: Planning for Future NNSA Experimental Facilities

ISSUE: Request that the laboratories follow the process developed by the "New Facilities Committee" (members nominated by the laboratory directors) for creating a

Laboratory. I want to personally thank this team for their insights and hard work in support of this important effort.

Similar to the 2003 Office of Science Twenty-Year Facility Plan, NNSA is exploring its decadal ST&E facility needs

- Science, Technology & Engineering (ST&E) has underpinned every stockpile decision and is required to assure continued Stockpile Stewardship Program (SSP) success
- Post-2020 mission drivers are more diverse and require renewed investment in ST&E infrastructure

ST&E is not done.
In fact, mission imperatives for ST&E are increasing.

Filling the gap in our ability to 'predict and control from materials and devices to manufacturing processes' is especially urgent

New Facilities Process Outcome:
"…we would expect to move MaRIE to CD-0 within 6 months"

Department of Energy
National Nuclear Security Administration
Washington, DC 20585

DEC 0 3 2012

MEMORANDUM FOR PARNEY ALBRIGHT
DIRECTOR, LAWRENCE LIVERMORE NATIONAL LABORATORY

PAUL HOMMERT
PRESIDENT AND DIRECTOR, SANDIA NATIONAL LABORATORIES

CHARLES McMILLAN
DIRECTOR, LOS ALAMOS NATIONAL LABORATORY

FROM: DONALD COOK
DEPUTY ADMINISTRATOR
FOR DEFENSE PROGRAMS

SUBJECT: Future Experimental Facilities: Decisions following the 2012 Review

Thank you for the efforts of your laboratories in planning for future experimental facilities supporting national security. Following my September 2011 request, the National Nuclear Security Administration (NNSA) national laboratories provided a roadmap and corresponding set of proposals that were uniformly outstanding. The great diversity of ideas reflected in the proposals is a testament to the dedication and quality of the technical communities at our laboratories.

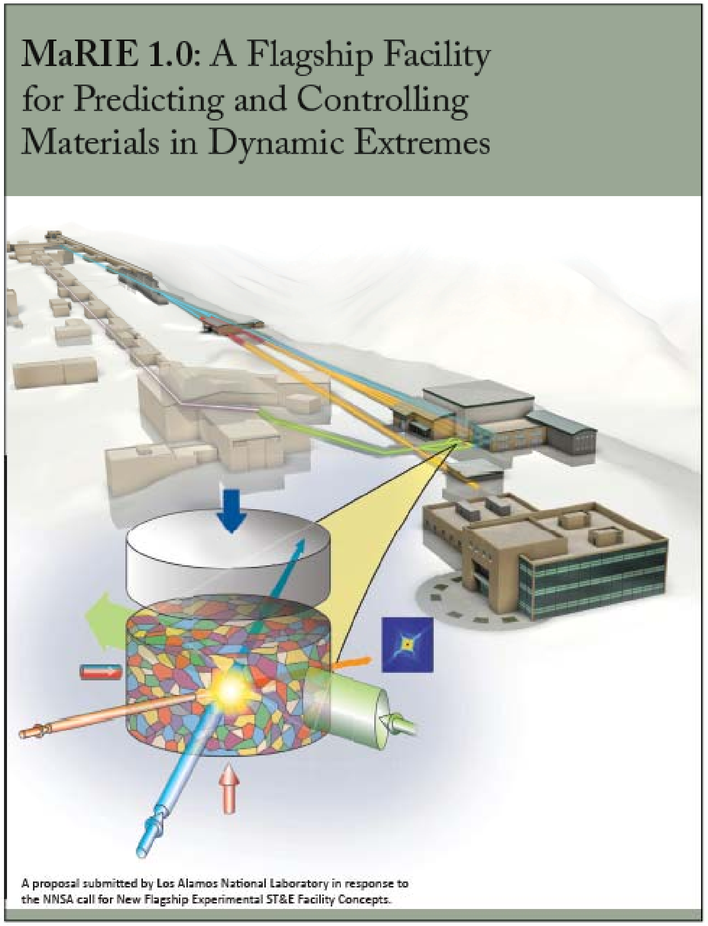
Our review of the plans for future experimental facilities benefitted from the contributions of independent experts. These experts are world leaders in science and engineering key to national security, individuals with extensive experience with the U.S. Department of Defense (DoD), and prominent leaders in NNSA's Stockpile Stewardship Program. These experts also have the technical depth and experience needed to understand the strategic value of the proposals advanced by the national laboratories. Input from each of these independent experts weighed considerably on our deliberations and decisions.

In the Tri-Laboratory Facility Roadmap submitted to Headquarters, you advanced a strategy focused on developing capabilities to:

"… predict and control from materials and devices to manufacturing processes."

- "MaRIE was, by far, judged to be the most mature and well-motivated proposed facility"
- "The cost estimate, schedule estimate, and technical feasibility of MaRIE are assessed to be at a level of fidelity beyond what is needed at this stage in the planning process"
- "The technical capabilities provided by MaRIE could substantially advance our ability to maintain the stockpile, but only if utilized within the appropriate framework."
- "Acceptance of MaRIE for CD-0 will require a letter from the directors of LANL and LLNL that describes your commitment and plan for advancing the process and science of certification to make use of MaRIE."

MaRIE 1.0 will enable us to observe and ultimately control how mesoscale materials properties affect weapons performance



A mission need exists for a facility focused on predicting and controlling materials in extreme environments, exploiting *in situ* transient measurements on real materials in relevant dynamic extremes to address key nuclear weapons challenges.

Achieving controlled functionality at the mesoscale through co-design is the **frontier of materials research**.

MaRIE 1.0 meets this need with a robust preconceptual reference design that is grounded in **community-defined mission and scientific requirements**.

LANL can realize MaRIE 1.0 by FY20 for a total project cost of ~ $1300M ($950M - $1800M).

MaRIE 1.0 is urgently needed to steward the stockpile and contribute to broader national security challenges early in the next decade