The Dynamic Mesoscale Materials Science Capability (DMMSC is the problem)
Formerly known as the Matter-Radiation Interactions in Extremes Project
(MaRIE could be the solution)

P/T Colloquium,
Cris W. Barnes
February 14, 2019

(stealing profusely from many others such as A. Bishop, J. Sarrao, B. Carlsten, R. Sheffield, and more!!)
The Dynamic Mesoscale Materials Science Capability (DMMSC) addresses a national unmet scientific need for understanding material performance and production at the mesoscale.

The ultimate goal is the integration of material structure and processing to achieve desired material properties and ultimately desired performance – supporting production science.

The MaRIE (Matter-Radiation Interactions in Extremes) Facility is one plausible solution that meets all the validated requirements for DMMSC.

The mission need for the capability and the facility project are important timely priorities for DOE/NNSA and Los Alamos National Laboratory.
To be a “Capture Manager” for a major, revolutionary, scientific capability, I try to be:

» Ludicrously Optimistic

» Patient

» Crazy

» Honest
Ludicrous Optimism!

LUDICROUS SPEED GO !!!
As scientists, we are all engaged in the grand journey of **Making History**

“Invention is the product of a creative or curious mind. **Innovation** is something that changes the life of our customers or their world.”

—Arno Penzias, Former VP, Bell Labs, Nobel Laureate
Designing Materials to Achieve Desired Performance is a Revolutionary Advance for Humanity
Tailored Materials at Work…
Thanks to Edwin Fohtung, NMSU
As a Laboratory, Los Alamos stewards broad and deep capabilities for multi-program leverage and benefit.

**Stockpile Stewardship**
- Detonator Safety, Performance in LEPs
  - Movies of functioning detonators

**Global Security**
- Microwave Technology
  - Electrically small antennae based on metamaterials concepts
- Center for Integrated Nanotechnologies (CINT)
  - Functional nanomaterials

**Energy Security**
- Perovskite Materials
  - Tailored material for sensors and collectors
- Flow Battery
  - New materials for energy generation, storage & transmission
Revolutionizing Materials in Extremes requires understanding material behavior at the Mesoscale

Atomic

Simple Perfect Homogeneous

10^{-10} 10^{-8}

Mesoscale

Emergent Phenomena

B field on (60 mT)

10^{-7} 10^{-6}

Internal features Interacting

Extreme Environments

10^{-7} 10^{-6}

Defects and Interfaces

10^{-5} 10^{-4}

Environments

phase separation

10^{-3} 10^{-2}

Interfaces

Continuum Bulk Behavior

 Macroscale

bulk

Wrought Cast

10^{-2} 10^{-1}
Understanding material structure-property-process relationships requires understanding the mesoscale


- Aging
- Manufacturing
- Material replacement
- Safety and surety

Nano-scale manufacturing and nanoscience integration.

- Pulsed laser deposition yields epitaxial metallic nanopillars integrated in oxide matrices
- Tunable densities on selected substrates yields controllable anisotropic optical properties
DMMSC will address the control of performance and production of materials for national security science at the mesoscale.

**Performance of additively-manufactured (AM) structural components**

- Wrought
- Annealed
- AM

Damage in wrought vs additively-manufactured steel

**High Explosive performance and safety**

Movies of functioning slapper detonators

**Requirement for MaRIE** are set from analysis of such experiments. -- "(U) MaRIE First Campaigns,” LA-CP-15-00501, June, 2015

**Void Collapse in energetic materials**

Identify mechanisms of initiation

**Ejecta and Mix**

Movies of ejecta in convergent geometry

DMMSC fills a critical gap in length scale between the integral scale addressed by DARHT and U1a and facilities such as NIF and Z.
Our **Science Pillars** define strategic capability investment areas at Los Alamos for present and future missions.

**Materials for the Future**
- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena

**Science of Signatures**
- Discover Signatures
- Revolutionize Measurements
- Forward Deployment

**Information, Science, and Technology for Prediction**
- Complex Networks
- Computational Co-Design
- *Data Science at Scale*

**Nuclear and Particle Futures**
- High Energy Density Physics & Fluid Dynamics
- Nuclear & Particle Physics, Astrophysics & Cosmology
- Applied Nuclear Science & Engineering
- Accelerators & Electrodynamics
The Matter-Radiation Interactions in Extremes (MaRIE) now DMMSC project has followed a rigorous pre-conceptual approach to meet mission and science challenges

» Benefit from the scientific community Workshops and studies surveying the decadal challenges for materials science.

» **Motivate** the science need for the mission through development of “First Campaigns”*

» Develop and **Justify** the scientific functional requirements by analysis of detailed “First Experiments” in each mission-relevant campaign

» Assert that a coherent, brilliant x-ray source that has energy and repetition rate characteristics matched to address materials performance challenges is required

Develop a pre-conceptual reference design, that can meet the requirements, with credible scope, cost and schedule estimates, and that can determine technical risks and define technology maturation plans.

*“(U) MaRIE First Campaigns,” LA-CP-15-00501

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

**Process-Aware Manufacturing First Campaigns**
- Old Materials: Aging
- New Materials: Controlled Functionality
- New Processes: Advanced and Additive Manufacturing
There is an envelope of common technical requirements on the probes to be able the make required measurements.

I apologize for not taking the time in this talk to walk through the justification for these functional requirements.

<table>
<thead>
<tr>
<th></th>
<th>Mission Need</th>
<th>Scientific Functional Requirements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spatial resolution</td>
<td>&lt;100 nm - 20 μm</td>
<td>&lt; 100 nm - 20 μm</td>
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<tr>
<td>Field of View</td>
<td></td>
<td>100 nm</td>
</tr>
<tr>
<td>Pu Casting</td>
<td></td>
<td>&lt; 1 μm – 100 μm</td>
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<td>Metals and Age</td>
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<td>aware performance</td>
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<td>HE certification</td>
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<tr>
<td>and qualification</td>
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<td>Turbulent Materials</td>
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<td>Mixing</td>
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<td>min pulse sep</td>
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<td>&lt; 500 psec</td>
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<tr>
<td>macropulse length</td>
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<td>sample thickness</td>
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<td>repetition rate</td>
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<td>lattice measurement</td>
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<tr>
<td>species</td>
<td>Be - Pu</td>
<td>Typically C, H, O, N</td>
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<tr>
<td>density</td>
<td>1%</td>
<td>3%</td>
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<tr>
<td></td>
<td></td>
<td>Noble gases, Ga, Be</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Pu</td>
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<td>0.1%</td>
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</table>
To see with time-dependence into and through the mesoscale requires: x-rays; coherent; brilliant and high repetition-rate; of sufficient high energy; and multiple probes at multiple scales.

DMMSC builds on the major technical revolutions in: **x-ray lasers** and their brilliance (for time-dependence); and **coherent imaging** (allowing high-resolution observation of non-periodic microstructure).

**“Ordered Light for Disordered Systems” – Paul Alivisatos**


**DMMSC Unique Complementary Characteristics:**
- Harder in energy for mesoscale, high-Z materials
- Higher in repetition rate to make movies of microstructure evolution
- Multiple probes to support maximum science return

The concept features multiple probes (x-rays, protons, electrons, optical photons) to maximize the science.
DMMSC (the Project) could provide the capability by building a 12-GeV electron linac feeding a 42-keV XFEL with experimental facilities.

Our pre-conceptual reference design would be located on the north side of the LANSCE mesa, leveraging the capabilities of that proton/neutron facility.

DOE is formally progressing through approvals in DOE Order 413.3B on the path towards a conceptual design.
DMMSC would fill a critical capability gap for dynamic (time-dependent) mesoscale materials science. DMMSC uses material samples that allow resolution of mesoscale science. DMMSC is positioned to deliver critical stockpile science data, filling a “knowledge gap” between existing facilities such as the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory and the Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) at Los Alamos.
Accelerator Capability has long been central to Los Alamos execution of mission.
DMMSC will complement the growing number of world-wide 4th generation light source capabilities.

"The United States had a significant fraction of all the world-leading capabilities 20 years ago, but that lead has eroded and today’s landscape is one of intense competition from both Europe and Asia."

Slide modified from Bob Cauble LLNL/HiBEF
Patience

My first P/T colloquium on “MaRIE” was nearly 10 years ago in June, 2009
Los Alamos has been working toward our vision of MaRIE since 2006 – a clear path is now defined!

- **Facility Definition** (2010)
- **Pre-conceptual Proposal** (2012)
- Setting the Stage for Mission (3/2014)
- “Move to CD-0” (2013)
- Submittal of CD-0 Package (5/2015)
- Need Approval of Pre-conceptual Mission Proposal (5/2015)
- Need for a Facility (3/2014)
- Project by Definition the Deputy Secretary (2014)
- **Developing the Energy Science Case** (2013)
- (2010)
- Validate Requirements (2018)
- Analysis of Alternatives (2019)
- Begin Conceptual Design (2020)

(3/2016) Formal Approval of the Mission Need for a Project by the Deputy Secretary of Energy
The acquisition of major capital projects by the DOE is governed by Order 413.3B and follows a series of “Critical Decisions”.

MaRIE has received CD-0 and is now on the Path to CD-1.
We developed a reasonably detailed design and cost estimate for the CD-0 Package.

The TPC for MaRIE was independently reviewed. Key lesson is we must avoid setting cost/schedule performance expectations too early! Cost Range in MNS is $1.9B-$3.7B.

Cost estimate is fully burdened with 38% average contingency.
LANL sees the future Weapon Science program supporting three major objectives; we envision a need for specific next-generation capabilities.

1. Complete PCF out-year pegposts
   - Primary performance, Secondary Performance, **Hostile Survivability**, Delivery Environments

2. Sustain an aging stockpile
   - How long will a weapon be viable? What is its lifetime?
   - Aging, Features

3. Enable stockpile responsiveness
   - What warhead options can be developed and certified?
   - Advanced Manufacturing, Features

From Michael Bernardin, ALDWP, May 2018
The Dynamic Mesoscale Materials Science Capability has been and continues to be central to the strategy for the future nuclear enterprise. We will deliver on commitments today while ensuring capabilities for an uncertain future. And integration of those capabilities is vital.
Craziness!

Arthur Clarke’s First Law:

When a distinguished but elderly scientist states that something is possible, he is almost certainly right. When he states that something is impossible, he is very probably wrong.
Unique Characteristic 1: High energy photons allow measuring bulk properties by maximizing elastic scattering for diffraction and minimizing absorptive heating.

The total (solid lines) and elastic (dashed lines) x-ray cross-sections as a function of incident photon energy for various materials

After suggestion by George Srajer, APS@ANL

Unique Characteristic 1: > 42 keV photons allow taking multiple images of high Z materials with an acceptable temperature rise.

A key design requirement, that will be central to balance of cost, risk, and performance, will be the fundamental x-ray energy.
DMMSC will address materials science needs at vastly different time scales

- **ps – ns**
  - Metastable electronic states

- **ns – 100 ns**
  - Phase Transformations

- **100 ns – 10 μs**
  - Shock transit across grain; Hydrodynamic instability

- **10 μs – 1 ms**
  - Shock transit across sample

- **10 s – 10 hour**
  - Thermal pulse evolution

- **months – years**
  - Additive manufacturing build

Key Requirement: a flexible linear accelerator pulse structure that can span from electronic/ionic (sub-ps) through acoustic (ns) to shock transit across samples (μs) to thermal (ms) to manufacturing (secs and above) event time scales.
Unique Characteristic 2: Time-dependent control of the mesoscale requires an innovative and flexible linac pulse structure that can span from electronic/ionic (sub-ps) through acoustic (ns) to shock transit (µs) to thermal (ms) event time scales.

Macropulses

MaRIE multiplexes 42-keV x-ray photons (blue), 12-GeV electrons (purple), and 0.8-GeV protons (red) during a single dynamic event.

Macropulse separation = (10 Hz)$^{-1}$

$T_{macro} = 69$ ns to $700$ µs (1 ms goal)

24.6 ns

40.6 MHz

10 fs to 100 fs

2.3 ns

30 pulse burst

Phase change

Deconstruction of sample

Unperturbed sample measurement

Ranges from sub-µs to 1 ms

Beginning of void formation

We plan on using an optical split and delay to generate sub-ns pulse separation.

Requirements on repetition-rate and duty cycle are also critical!
Unique characteristic #3: The need for multiple probes is driven by science

» Phase response under failure (Bronkhorst)
  » Broad field-of-view to determine shock location, rarefaction waves, gross grain motion
  » Narrow x-ray field-of-view to measure phase and grain plastic response

» Ejecta evolution from Richtmyer-Meshkov jetting (Bolme)
  » Broad field-of-view to determine bulk fluid motion and vorticity
  » Narrow x-ray field-of-view to scatter off ejecta and determine phase and structure evolution
DMMSC will provide critical data to inform and validate advanced modeling and simulation to accelerate qualification of advanced manufacturing – move from “process-” to “product-based”

DMMSC and Exascale will enable rapid and confident deployment of new concepts and components through more cost-effective and more rigorous science-based approaches.

Microstructure

Properties

Performance
The “broader sense of co-design”: How fast can we iterate around this process?

- The experiments can now be done “rapidly” (every few minutes to 120 Hz! And faster coming!!)
- The issue of “data science” is actively being attacked.
  - Including Real-time simulation and decision-making
- Rate-limiting step is, or is about to be, “adaptive target fabrication”
  - 1 Hz experiment in 8-hour shift can be >20,000 targets!!

The Revolution is Hard! I claim it will be worthwhile!
Sample preparation (aka target fabrication) may, after data acquisition and analysis (aka data science), be rate-limiting step to high-throughput materials science.

High-repetition-rate brilliant and coherent light sources are significantly increasing the rate at which scientific experiments can be performed. In fields of molecular biology and chemistry, fluidic methods allow large numbers of samples to be prepared. Major investments in data science and machine learning are reducing the bottlenecks on data acquisition and analysis. A concomitant investment in transformative technologies to make condensed matter materials samples could enable a paradigm shift for that field as well.

John Oertel and others are organizing a workshop at Texas A&M in mid-May on “Adaptive Sample Preparation and Target Fabrication for High-Throughput Materials Science”
MaRIE is a plausible facility solution that meets the DMMSC requirements – And it will be a revolutionary capability!

» The brilliance of an XFEL

» Transformative imaging techniques with coherence – “ordered light for disordered systems”

» Designed for time-dependence from electronic motion (picosecond) through sound waves (nanosecond) through shock transit across samples (microseconds) through thermal diffusion (millisecond) to manufacturing (seconds and above)

» High-energy to not destroy mesoscale samples with that brilliance and give that time-dependence (and perhaps provide larger reciprocal space resolution)

» Not just x-ray facility, but designed for multiple simultaneous probes

» Designed with strong connection to the needs of scientific predictive capability from theory, modeling, and computation

» Providing comprehensive materials discovery capability to collaborative teams

» Enables science-based qualification and certification, leading to the “revolution in manufacturing/production science”
Maybe I’m not so crazy: Some quotes from the just-published Materials Decadal Report, 2019

Key Recommendation: Federal agencies (including NSF and DOE) with missions aligned with the advancement of additive manufacturing and other modes of digitally controlled manufacturing should by 2020 expand investments in materials research for automated materials manufacturing. The increased investments should be across the multiple disciplines that support automated materials synthesis and manufacturing. These range from the most fundamental research to product realization, including experimental and modeling capabilities enabled by advances in computing, to achieve the aim that by 2030 the United States is the leader in the field.

Key Recommendation: The U.S. government, with NSF, DOD, and DOE coordinating, should support the quest to develop new computational and advanced data-analytic methods, invent new experimental tools to probe the properties of materials, and design novel synthesis and processing methods. The effort should be accelerated from today’s levels through judicious agency investments and continue over the next decade in order to sustain U.S. competitiveness.

A principal development of the last decade has been the emergence of X-ray free electron lasers as a complement to synchrotrons, notably the Linac Coherent Light Source (LCLS) and the future LCLSII and its high-energy upgrade, LCLS-II-HE, at SLAC in the United States. New X-ray free electron lasers have been built or are under construction at DESY (Germany), PSI (Switzerland), CAS Shanghai (China), and elsewhere.

Collectively, these new ultrabright sources will drive further advances in the techniques, enabling transformative studies of materials with nanoscale resolution while under operating conditions and on ultrafast time scales. The United States had a significant fraction of all the world-leading capabilities 20 years ago, but that lead has eroded and today’s landscape is one of intense competition from both Europe and Asia.

The broad photon energy range available (from the far IR to hard X ray) and the intense brightness of the beams, which allows the photon beams to be tailored to specific experimental geometries and environments, makes X-ray light sources near-ideal probes of the structure and function of materials. As the field moves toward the capability to fully integrate computational materials science, synthesis, and advanced manufacturing for real-world performance, the microscopic characterization of structure and dynamics enabled by the next generation of instruments and upgraded sources will provide the crucial link to enable materials by design.
Honesty
LANL staff should care about MaRIE in 2009 (a slide from February 2009, 10 years ago)

» MaRIE strongly support LANSCE’s central role in the Lab mission
  » (LANSCE-Refurbishment, Enhanced Lujan Neutron Scattering Center, Materials Test Station for fission energy science)

» MaRIE enables our Materials Strategy
  » It engages us in key national directions of material science
    » We become leaders in the transformation from the “era of observation” to the “era of control” and providers of “functionality by design”
  » It provides resources to enable strategic investment in the LANL Materials Strategy
    » Guides LDRD, provides enabling R&D support, and can re-direct programmatic interest

» MaRIE is an experimental facility
  » It can transform non-materials science at Los Alamos
  » It will enhance LANL capabilities for all our customers
  » 30 years from now its use will be different – just as with LAMPF
Conclusion

» Big, great things take time – lots of time

» They are worth doing (“Do or do not, there is no try”)

» I hope you will help us achieve this vision of a great future for our Lab.
The Dynamic Mesoscale Materials Science Capability (DMMSC) addresses a national unmet scientific need for understanding material performance and production at the mesoscale.

The ultimate goal is the integration of material structure and processing to achieve desired material properties and ultimately desired performance – supporting production science.

The mission need for the capability and the facility project are important timely priorities for DOE/NNSA and Los Alamos National Laboratory.

Understanding process-structure-property-performance relationships requires a research capability to explore mesoscale dynamics.
<table>
<thead>
<tr>
<th>Hard X-ray FEL Parameters</th>
<th>LCLS-I</th>
<th>SACL A</th>
<th>EXFEL</th>
<th>PAL XFEL</th>
<th>SwissFEL</th>
<th>LCLS-II</th>
<th>LCLS- MaRIE</th>
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<tr>
<td>X-ray energy</td>
<td>12.8 keV</td>
<td>19.5 keV</td>
<td>24.7 keV</td>
<td>20.6 keV</td>
<td>12.4 keV</td>
<td>5 / 25 keV</td>
<td>15 keV</td>
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<td>Pulse energy</td>
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<td>0.03 mJ</td>
<td>1 mJ</td>
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<td>1.4 mJ</td>
<td>0.025 / 0.3 mJ</td>
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<td>&lt;1 μs 60 Hz</td>
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<td>CW / &lt;1 μs 930 kHz / 120 Hz</td>
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<td>1-2</td>
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<td>2,700</td>
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<td>N/A (CW) / 1-2</td>
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<td>200 pC</td>
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<td>0.6 μm</td>
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