





## Center for Radiative Shock Hydrodynamics (CRASH)

**Overview** 

**R.** Paul Drake, Project Director



## Outline



- Big picture background for CRASH
- The experimental program
- The structure of our calculation
- Our coding practices
- Our approach to uncertainty quantification
- Our Co-Pls
  - James Holloway (Nuclear, UM)
  - Ken Powell (Aerospace, UM)
  - Quentin Stout (Computer Science, UM)
  - Marvin Adams (Nuclear, TAMU)

### The very big picture for this project



- Based on established and successful codes
  - BATS-R-US (widely used, 15-year track record) for hydro
  - PDT code from TAMU for radtran
  - Space Weather Modeling Framework (SWMF) for coupling
- Based on the Michigan system of software development
  - A core research scientist team orbited by method developers and code users
- Based on development of methods and software for assessment of predictive capability
- Based on a flourishing experimental program

We are poised to provide tools that will have major impact on university science at major NNSA facilities

## Our goal is to understand radiative shocks and how well we can predict their behavior

- Radiative shocks have structure that is strongly affected by radiative energy transport
- Complex axial and lateral structure
- Simulations need coupled 3D hydrodynamics, radiation, other physics



**Axial structure** 

Lateral structure

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## Two key dimensionless parameters for radiative shocks involve optical depth





## The other key parameter relates to shock velocity



- Any sufficiently fast shock becomes radiative
  - Once the upstream radiation from the shock exceeds the incoming mechanical energy flux:

$$R = \frac{oT^{4}}{\rho_{o}u_{s}^{3}/2} > 1 \qquad T \propto u_{s}^{2} \qquad R \propto \frac{u_{s}^{5}}{\rho_{o}}$$

- This takes ~ 50 km/s shock waves in xenon at 1 atm.
- It takes ~ 200 km/s in CH foam at ~ 10 mg/cc



### Hard is good

- We chose not to propose a simple validation problem in which one more-or-less knows all the answers
- Why not?
  - The real need for creativity and innovation will be found in the hard problems, not the easy ones
  - The problems the NNSA labs need to address are hard indeed









-C/L

ZBL Laser

LANL experiment At Z

NIF: LLNL Drake Overview Talk

Page 8

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### Our problem is in the area of high-energydensity physics



- The study of ionized matter having pressures near or above
   1 Mbar, and of the methods of producing such matter
- This is the regime in which solids are compressible
- HEDP matters to NNSA
  - The core problems of interest to NNSA are in the HEDP regime

Radiative shocks are one of the fundamental phenomena occurring in HEDP systems



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## **High-Energy-Density Physics is fun too**



#### We make amazing numbers in the lab!



Laser-driven shock wave

#### The "Z" Machine fires

Shock waves that travel > 300 km/s

Temperatures of hundreds of eV



#### The Omega laser strikes



Pressures of 100 million atmospheres by laser ablation

#### Megajoules of X-rays

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# HEDP has also been attracting increasing national interest



**1.** National Research Council, *Connecting Quarks with the Cosmos*: Eleven Science Questions for the New Century (Quarks to Cosmos), National Academies Press, Washington, DC, 2003.

**2.** The Science and Applications of Ultrafast, Ultraintense Lasers (SAUUL): Opportunities in Science and Technology Using the Brightest Light Known to Man, Report on the SAUUL workshop sponsored by DOE and the National Science Foundation (NSF), 2002.

**3.** National Research Council, *High Energy Density Physics*: The X-Games of Contemporary Science (HEDP/X-Games), National Academies Press, Washington, DC, 2003.

4. National Science and Technology Council Committee on Science, A 21<sub>st</sub> Century Frontier of Discovery: **The Physics of the Universe** (2004-POU), **Office of Science and Technology Policy**, Washington, DC, 2004.

5. National Task Force on High Energy Density Physics, *Frontiers for Discovery in High Energy Density Physics* (Frontiers for Discovery in HEDP), Office of Science and Technology Policy, Washington DC, 2004.

### Our problem is also relevant to astrophysics



- HEDP has much in common with some astrophysical systems
  - Very-high-Mach-number shocks
  - lonized media
  - Strongly compressible behavior
  - Radiation-dominated energy flow

Kifonidis: ApJ 03



Examples: Supernovae and supernova remnants



#### **Our very successful HEDLA conference has run since 1996**

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#### Our experiments have the same three relevant dimensionless parameters as shocks emerging from supernovae **Ensman & Burrows ApJ92**



- **Optically thin upstream**
- **Optically thick downstream**
- Large ratio of radiative to mechanical energy fluxes
- This produces qualitatively similar profiles
  - If there is important unanticipated physics, we may see it
  - Good code test in any event



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## Unanticipated physics can happen



- Results from our recent supernova hydrodynamics experiments
- Blast-wave-driven interface instabilities show unanticipated tendrils of mass ahead of the Rayleigh-Taylor spikes



#### mid-90's

• Seeing this required our improved diagnostics

## Our experimental program provides advanced technical training in a team environment

- The photos show
  - A meeting to discuss upcoming projects involving our x-ray source and microchannel plates



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A meeting to discuss target design and construction for experiments at Omega



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Page 15

## Current and recent experimental graduate students

**Forrest Doss** 



Dr. Amy Reighard (@ LLNL)



**Carolyn Kuranz** 



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#### **Eric Harding**

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Christine Christine Krauland Tony Visco Chan Huntington

Page 16

#### We collaborate very extensively

#### **Collaborators:**

LLNL – Remington, Robey, Miles, Edwards, Hansen, Froula, others France – Bouquet, Koenig, Michaut, Busquet LLE/Rochester – Knauer, Boehly Arizona – Arnett Chicago – Hearn, Meakin Stony Brook – Glimm, Swesty NRL – Aglitskiy, Weaver

Texas – *Wheeler, Ditmire* Florida State – *Plewa* 



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# The experimental program has current projects in several areas relevant to CRASH



- Blast-wave driven instabilities
- On Omega –
- On NIF
- Kelvin Helmholtz
  - Relevant to astrophysics and ICF
  - On NIKE and Omega
- Radiative shocks
  - Interesting objects !
  - Astrophysically relevant
  - On Omega
  - On LIL collaborating with team led by Claire Michaut
- X-ray diagnostics







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# What we do at Michigan in the experimental program

- At Michigan we
  - Design experiments and measurements
  - Simulate experiments
  - Analyze data
  - Do some instrumentation research
  - and .....

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- We build targets
  - Great educational value
  - Rapid innovation
  - Division of labor (grad/undergrad)
- We then go to laser facilities for experiments





Page 19

### **Evolution of radiative shock targets**





### How we produce radiative shocks



Laser beams launch Be piston into Xe or Ar gas at > 100 km/s

**Piston drives a planar shock** 

Radiography detects dense xenon

Gold grid provides spatial reference

600  $\mu$ m tube dia.

Parameters 10<sup>15</sup> W/cm<sup>2</sup> 0.35 µm light 1 ns pulse 
 Ne filled tube

 Grid

**Experiments: Amy Reighard** 

10 drive beams

**Strike Be disk** 

#### Targets: Mike Grosskopf, Trisha Donajkowski, Donna Marion, Mark Taylor

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Page 21

## Radiographs provide the core data for quantitative comparison to simulation output





## Other diagnostics will provide additional data

- Data from experiment with average velocity 140 km/sec through 14.6 ns
- See A. Reighard *et al.* 
  - Phys. Plas. 2006, 2007
- Details for quantitative comparison with simulations
  - Shock position at data time
  - Average thickness of Xe layer
  - Average curvature of front and rear surface
  - RMS deviation of front and rear surface from average shape
  - Distance of edge of shock from tube wall
  - Average thickness of trailing feature
  - Distortion of tube wall vs distance from shock

# Simulations using the LLNL code HYDRA explored the structure near the edge





Radiation from the shock induces plastic ablation, radial blast wave in the tube

Primary shock meets wall shock inducing obliqueness

Wall shock features:

- Dense Xe collected behind the primary shock
- Curvature of the trails
- Edge displacement
- Angle

Simulations: Forrest Doss Page 23

## Lateral structure may result from a Vishniaclike mechanism. Simple Vishniac:





## Theoretical analysis shows structure internal to shocked layer for the experimental case



- Wavelength and growth rate of maximum instability in reasonable agreement with experimental observations
- Stereoscopic experiments this week will seek further evidence

Drake Overview Talk Theory by F. Doss Page 25

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## **Our signature Year 5 experiment**



- The Year 5 experiment will be an experiment that is identical except that the shock tube cross section is an oval with an aspect ratio of 2 to 1.
  - This is a 3D system
  - The variation in radiation irradiance as azimuthal angle varies is ~ 30%
  - Likely to affect features near wall
  - We will take two perpendicular views of radiography data, along the short and long axes
- How different is the signature experiment from the component experiments leading up to it?
  - The difference is the shape of the tube wall; this introduces 3D structure.

## In software we are very much building on our experience

- Successes with codes
  - An adaptive 3D (routine!) MHD code
  - Coupled models run under a framework
  - Realistic radiative transfer
  - Successes with large calculations
  - Management and implementation of large massively parallel calculations
- We have a rich computational science environment at UM
- We anticipate spinoffs from this project to other UM research
  - Flux emergence from the radiative solar photosphere
  - Modeling of high-Mach-number hydrodynamic experiments
  - Coupled physics engineering models





# Our software system will build on three major existing packages



#### • These are

- **BATS-R-US**: high performance MHD developed at UM
- PDT: Parallel Deterministic Transport, developed at TAMU, uses STAPL (Standard Template Adaptive Parallel Library)
- SWMF: Space Weather Modeling Framework, developed at UM with software engineering oversight by NASA
  - Widely used through the Community Coordinated Modeling Center at Goddard
- Software for assessment of predictive capability will be new

### Our codes are Mature but not Old



- Mature: UM & TAMU have extensive experience running these codes on wide range of platforms: clusters, Cray T series, SGI shared-memory, BlueGene/L, ...
- Not Legacy: developed from the ground up to run on large parallel systems, using modern software development techniques and standards.
  - SWMF and BATS-R-US in Fortran 90 + Perl
  - PDT and STAPL in C++
  - All
    - are object-oriented
    - use standard naming conventions
    - have rigorous testing procedures
    - generate documentation automatically, etc.

## BATSRUS solves hydrodynamic equations with source terms

Nonlinear conservation laws for state W driven by source S

$$\frac{\partial \mathbf{v}}{\partial t} + (\nabla \bullet \mathbf{G})^{T} = \mathbf{S},$$

$$\mathbf{W} = \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \\ \varepsilon + \frac{1}{2}\rho u^{2} \\ \varepsilon_{e} \end{pmatrix} \qquad \mathbf{G} = \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} + p\mathbf{I} \\ \mathbf{u} \left(\varepsilon + \frac{1}{2}\rho u^{2} + p\right) \\ \mathbf{u} \varepsilon_{e} \end{pmatrix}^{T} \qquad \begin{array}{l} \text{Density} \\ \text{Momentum} \\ \text{Fluid Energy} \\ \text{Electron Thermal} \\ \text{Energy} \end{array}$$

**DAT** 

Closed with equation of state (EOS) relationships

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### **BATS-R-US is a Multi-Physics Code**



- Compressible fluid dynamics
- Ideal MHD
- Resistive MHD
  - Resistivity models are poorly understood
  - Numerical resistivity often dominates
- Hall MHD
  - Keeps the Hall term in Ohm's law
  - More realistic reconnection rate
- Semi-relativistic MHD
  - Displacement current in Ampère's law
  - Limits all wave speeds by c
- Physics-based energy transport
  - Heat conduction
  - Wave energy transport
- Multi-fluid MHD
  - Each ionic species has its own continuity, momentum and energy equation
  - Electron momentum equation is replaced by Ohm's law.
- Goal: semi-relativistic, multi-fluid Hall MHD with anisotropic pressure.
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## **SWMF Superstructure and Infrastructure**



User Interface Layer	Web based Graphical User Interface configuration, problem setup, job submission job monitoring, result visualization	Ha tim
Superstructure Layer	Framework Services component registration, input/output execution control, coupling toolkit Component Interface component wrappers and couplers	ad
Physics Module Layer	SC BATSRUS Kota RCM	A
Infrastructure Layer	Utilities physics constants, time and date conversion coordinate transformation, field line tracing parameter reading, I/O units, profiling	n

Has evolved over time, features added as needed.

#### Added when Rice Convection Model made a component

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### SWMF simulation of a coronal mass ejection





## SWMF has been validated on magnetospheric data



- In late October and early November 2003 a series of some of the most powerful solar eruptions ever registered occurred.
- Halloween storm simulation provided a unique opportunity for data comparison



## For CRASH, most hydrodynamic source terms come from radiation transport





Radiation/Electron Momentum Exchange Electron Conduction & Radiation/Electron Energy Exchange

Electron thermal energy source

**Electron energy source term:** 



## PDT solves the radiation transport equation



• Intensity as function of space, time, frequency and direction

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla I + \sigma I = Q(I,\rho,\mathbf{u},T_e)$$

Moments over direction and frequency yield energy and momentum conservation

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{F} = S_{re} \qquad \frac{1}{c^2} \frac{\partial \mathbf{F}}{\partial t} + \nabla \cdot \mathbf{P} = S_{rm} \\ \int_{4\pi} \int_0^\infty \left[ -\sigma I + Q \right] d\Omega d\nu \qquad (1/c) \int_{4\pi} d\Omega \int_0^\infty d\nu \left[ -\sigma I + Q \right] \Omega \\ \text{contribution to electron thermal energy}$$

Neglect line emission & absorption and neglect scattering

## The material types and properties also matter



- Code designed to support variety of EOS formulations
  - Ideal gas, In-line formulations, Tabular EOS
- Thermal emission, first grey then multigroup
- Track material boundaries to account for EOS, ionization, and opacity changes
  - Track using a zero level set approach
  - Advect the level set function
  - Hydro grid refinement to follow interface accurately

## For material tracking we plan to use level sets with AMR



- Zero level set contour encloses a particular material
- Does not provide exact mass conservation of the species
- Loss of species conservation controlled by AMR at the interfaces
  - Mesh used for level set can be refined independently of hydro mesh



### We will initialize our calculation with HYADES



- Laser package with 3D rays
- 2D Lagrangian code
- One set of continuity and momentum equations
- Multiple energy equations
- Flux-limited electron heat transport
- Multigroup radiation transport based on an average atom model

## HYADES model of hydrodynamic experiment at 1.2 ns



## **Our Integrated Calculation**



- Integrate existing hydro and radiation transport packages
- Provide robust initial implementation for predictive science
- Allow for implementation of more advanced rad-hydro coupling schemes



## **Computational requirements for coupling**



- Rad transport dominates time
  - 100x100x100 grid
  - hundreds of directions
  - $\rightarrow 10^8$  phase-space cells for each energy
  - tens of energies; minimum 10<sup>9</sup> variables
  - requires sweeps through all of space
- Hydro uses
  - far more spatial resolution, especially in highly resolved regions → 10<sup>7</sup> cells adaptive
  - dynamic adaptation and load balancing
  - spatially local communication
- Fortunately, rad/hydro coupling requires only a few quantities per hydro cell
  - hydro state variables
  - rad quantities integrated over direction and energy



- Modify PDT and integrate into SWMF
- The dominant effort: expand capabilities of components
   and coupled components
  - multiple large subprojects and new science
  - continually test and develop verification tests for components and coupled systems
  - maintain software development and documentation standards
- Expand superstructure and infrastructure as needed
- Attain high performance on platforms as they become available
  - improve performance bottleneck areas
  - identify strategies to simplify tuning on new platforms

### **Version Control**



- Use Concurrent Versioning System (CVS)
  - The CVS repository is backed up nightly
  - Separate repositories for BATSRUS and PDT
- Use a single development version (CVS HEAD)
  - Multiple branches are found to be counter-productive
- Tag versions before and after major changes
  - Helps recovering working versions, helps debugging
- Latest production version is kept close to development version
  - Allows fast utilization of new features and bug fixes
  - Allows fast discovery of bugs and design errors
- Multiple production versions for various classes of users

## **Nightly SWMF Tests**



#### **Machines and compilers**

name	platform	compiler	MPI run
grid/nag	Linux PC	NAG F95 v5.0(322)	mpirun -np 2
mesh/ifort	Mac with 2 dual-core Intel CPUs	ifort Version 10.0 beta	mpirun -np 4
grendel/nag	Linux cluster	NAG F95 v4.0a(388)	serial run
nyx/nag	Linux cluster with quad-core CPUs	NAG F95 v5.0(414)	serial run
xena/nag	Mac OSX cluster	NAG F95 v5.0(367)	mpirun -np 2
xena/xlf	Mac OSX cluster	XLF90 v8.1 beta	mpirun -np 2
columbia/ifor	sGI Altix system	ifort for Itanium v10.0-beta (20070307)	mpirun -np 4

#### **Test Results**

- · Red text shows what failed in a test.
- · Green text indicates that a test passed.
- · CAPITALIZED text shows results that have changed.
- Click on the machine name, the failed tests, or the log files for more info.

test / machine	<u>columbia</u>	grendel	grid	mesh	<u>nyx</u>	xena	xena xlf
GM/BATSRUS/test_corona	PASSED	passed	passed	passed	passed	passed	<u>RUN</u>
GM/BATSRUS/test_func	PASSED	1 test	passed	passed	<u>1 test</u>	1 test	3 tests
GM/BATSRUS/test_mars	PASSED	passed	passed	passed	passed	passed	<u>result</u>
GM/BATSRUS/test_multifluid	PASSED	passed	passed	passed	passed	<u>compile</u>	passed
GM/BATSRUS/test_multiion	PASSED	passed	passed	passed	passed	<u>compile</u>	passed
GM/BATSRUS/test_shocktube	PASSED	passed	passed	passed	passed	<u>compile</u>	passed
GM/BATSRUS/test_titan	PASSED	passed	passed	passed	passed	passed	passed
GM/BATSRUS/test_titan_restart	PASSED	passed	passed	passed	passed	passed	passed
GM/BATSRUS/test_venus	PASSED	passed	passed	passed	passed	passed	passed



# Our software development standards (34 pages) guide our work



- Use agile programming
  - Initial overall design is still used
- New self-contained program units are developed with unit tests
  - Unit tests must be complete and run in seconds
  - Code simplification (refactoring) is done after unit tests pass
- New features are implemented together with new tests
  - Tests must cover all aspects of the new feature
  - Use grid convergence studies, manufactured solutions and model comparison to verify new numerical algorithms
- Add or extend functionality test suite to fully check new feature
  - (use coverage tools) and its compatibility with existing features

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Page 46

## How will we know we have succeeded in assessing predictive capability?



#### • Success will be measured by

- The degree to which the comparison of measurements from the year-5 experiments against the preshot simulation results is consistent with the assessment of predictive capability
- The degree to which our inference system enables us over time to improve predictive capability
- Achieving nice "viewgraph norms" is far from sufficient
  - From past experience we are confident about quickly getting the approximate morphology

65 ns39 ns

Data

CALE PROMETHEUS

### We must go beyond traditional V&V and UQ



After this, must assess *predictive* capability for *next* event.

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## **Components of Assessment of Predictive Capability**

- Software quality assurance and verification
- **Propagation of input U's to output variations** 
  - Gives <u>code's</u> sensitivity (not necessarily nature's)
  - Part of "UQ" (which is part of "QMU")
  - Includes uncertainties:
    - In physical data
    - In initial & boundary conditions
- Estimation of numerical errors; propagation to output variations
- Assessment of measurement uncertainties and errors
- Inference of:
  - reduced U's in physical data
  - model error
- Quantitative assessment of predictive accuracy for NEXT event or experiment

#### Epistemic vs. aleatory uncertainties [ignorance vs. true variability]



- <u>Scenario 1: true variability dominates</u>
  - In this hypothetical limit, weapon performance is:
    - insensitive to our uncertainties in physical data
    - sensitive to as-built variations in stockpile.
  - Analysis says 90% of weapons in stockpile will meet requirements and 10% will not.
  - This 90% is a reliability number. It represents true variability.
- Scenario 2: ignorance dominates
  - In this hypothetical limit, weapon performance is:
    - sensitive to our uncertainties in physical data or correct models
    - insensitive to as-built variations in stockpile (all work or all fail!)
  - Analysis says 90% of input-space samples produce required performance; 10% do not.
  - This 90% is a confidence number. It represents our ignorance.
- Our analyses must keep these separate!

## Inference should be systematic & transparent



- Primary tool will be a Bayesian Hierarchical System
  - Builds posterior input-parameter distributions
  - Builds model-discrepancy function



• We also have an adjoint methods expert on our team and will pursue these methods too, in particular to guide grid refinement

### **Inference System: Advances**



- Advance: quantify sensitivity of Bayesian inferences to initial assumptions (e.g., "prior" distributions of inputs)
  - This can be done with no additional simulation runs
- Advance: use Bayesian machinery to produce posterior intervals instead of distributions (much less costly)
- Advance: further develop model-discrepancy function
  - try to quantify error in each physics model

## Quantitative assessment of predictive accuracy for NEXT event or experiment.



- This is an area for intense research.
- We will explore all avenues, including the rigorous-bounds approach recently devised by Lucas, Owhadi, and Ortiz.
- How do we know if the next experiment is "similar enough" to the ones we've analyzed before?
  - Rigorous metrics of "distance" between problems can help
  - Sounds questionable, but if used intelligently these metrics can offer real information
  - Will not eliminate physics knowledge & judgment

# We expect to create and apply significant advances in predictive science



- Our APC system will be comprehensive. It will include:
  - all source of simulation U
  - estimation of numerical errors
  - inference of model errors
  - inference of reduced physical-data uncertainties
  - continued learning as more data becomes available
- We expect advances in
  - dimension reduction for large correlated data sets
  - error estimation for hyperbolic systems
  - inference of model errors
  - combination of Bayesian and other approaches
  - quantification of sensitivity to initial assumptions
  - efficiency (reduced requirement for full simulation)

### **CRASH** is underway



- Actively hiring the 4 research scientists who are essential to getting the work done
  - Key to beginning implementation of uncertainty quantification
- Actively recruiting grad students
  - Approximately 15 at UM and 4 at TAMU working on CRASH projects this next AY
- Making progress on adaptation of PDT, and on BATSRUS hydro models and inline EOS
- Preparing for first dedicated CRASH experiments
  - This fall; focused on experimental variability
  - Other complementary experiments taking place this week

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Page 55