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Experiment A validation of the SURFplus High Explosive Model

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A Verification and Validation Study of the Cyclops I PBX 9502 Experiment

A validation of the SURFplus High Explosive
Model

John W. Grove

CCS-2

Tuesday, July 23, 2019

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The SURFplus Model

SURF: Burn initiation

- SURF is an acronym for Scaled-Unified-Reactive-Front
  - Invented by R. Menikoff and S. Shaw
- What follows is a brief synopsis of this model as used for the validation study discussed here. For more details see the xrage user manual and the references cited there.
- SURF and SURFplus are members of a broad category of reactive burn models that use the ignition and growth concept
- The burn front is detected using the Hugoniot function

$$H = e - e_0 - \left[\frac{P + P_0}{2} \right] (V_0 - V)$$

- The zero subscript corresponds to the state of the undisturbed explosive
    - The quantity H is identically zero in this region
  - Shock detection is initiated when H becomes positive
  - The lead shock is detected when H changes sign or pressure or density decrease
  - When a shock is detected in a cell the value P_{sh} is set, which is subsequently advected by the flow $\frac{DP_{sh}}{Dt} = 0$.
- For more details on the shock detection algorithm see
  - R. Menikoff. Shock detector for SURF model. Technical Report LA-UR-16-20116, Los Alamos National Lab., 2016.
URL <http://www.osti.gov/scitech/servlets/purl/1234496>.

SURF: Burn propagation

- Once the shock detector is activated burn is propagated by the equation

$$\lambda = g(s)$$

where λ is the reaction progress variable (mass fraction of the reaction products), $g(s)$ is a reaction-scale function and s is a dimensionless reaction-scale variable

$$\frac{Ds}{Dt} = f(p_{sh}) \begin{cases} 0, & p \leq 0 \\ \left[\frac{p}{p_{sh}} \right]^n, & 0 < p < p_{sh} \\ \left[\frac{p}{p_{sh}} \right]^{n_{hi}}, & p_{sh} \leq p \end{cases}$$

- The reaction-scale function is given by

$$g(s) = \frac{1}{g_n(s_1)} \begin{cases} g_0(s), & s \leq s_1 \\ g_0(s_1) + g'_0(s_1)(s - s_1) + \frac{1}{2} g''_0(s_1)(s - s_1)^2, & s_1 < s < s_{cutoff} \\ g_n(s_1), & s > s_{cutoff} \end{cases}$$

$$g_0(s) = 1 - e^{-s^2}$$

$$g_n(s_1) = g_0(s_1) - \frac{1}{2} \frac{[g'_0(s_1)]^2}{g''_0(s_1)}, s_{cutoff} = s_1 - g'_0(s_1)/g''_0(s_1)$$

- These formulas introduce three dimensionless parameters for the reaction scale evolution equation and the reaction-scale function: n , n_{hi} , and s_1

SURF: Shock-Strength Function

- The shock-strength function in the evolution equation for the reaction

scale function used the formula $f(p_{sh}) = \frac{\hat{f}\left(\frac{p_{sh}}{p_{scale}}\right)}{t_{scale}}$

$$\hat{f}(P_{sh}) = C \begin{cases} 0 & P_{sh} \leq P_0 \\ P_{low}^{f_n} \left[\frac{P_{sh} - P_0}{P_{low} - P_0} \right]^{1 - \frac{P_0}{P_{low}}} f_n & P_0 < P_{sh} \leq P_{low} \\ P_{sh}^{f_n} & P_{low} < P_{sh} \leq P_1 \\ P_1^{f_n} \exp \left[f_n \log\left(\frac{P_{sh}}{P_1}\right) \cdot \left(1 - \left[2 \log\left(\frac{P_{high}}{P_1}\right)\right]^{-1} \log\left(\frac{P_{sh}}{P_1}\right)\right) \right] & P_1 < P_{sh} \leq P_{high} \\ P_1^{f_n} \exp \left[\frac{1}{2} f_n \log\left(\frac{P_{high}}{P_1}\right) \right] & P_{high} < P_{sh} \end{cases}$$

- $f(p_{sh})$ is set to zero if the shock detector has not activated unless $p_{sh} > p_{burn}$ in which case burn will be initiated
- This function is defined by six dimensionless parameters and the pressure scale
 $C, P_0 = p_0/p_{scale}, P_{low} = p_{low}/p_{scale}, P_1 = p_1/p_{scale}, P_{high} = p_{high}/p_{scale}, f_n$
- Input for xRage uses these dimensionless parameters

SURF: Parameter Values used for PBX-9502

- The table below summarizes the values for the SURF setup for PBX 9502

Parameter	Value	Parameter	Value	Parameter	Value
t_{scale}	$1 \mu sec$	s_1	2.0	P_1	28.0
p_{scale}	$1 GPa$	C	4.6×10^{-5}	P_{high}	60.0
n	3.2	P_0	6.0	f_n	4.05
n_{hi}	0	P_{low}	8.0	p_{burn}	$25 Gpa$

- For the simulations in this study no addition energy release was added for the SURF model. The reaction energy release was embedded in the products equation of state

SURF: Model Curves

- The figures below show the graphs of the reaction-scale function and shock-strength function used by the SURF model. The curves used the parameters from the table on the previous slide.
- The sections of the curves are color coded by region
  - Reaction Scale Function: red $s \leq s_1$, blue $s_1 < s \leq s_{cutoff}$
  - Shock-Strength Function: black $\frac{p_{sh}}{p_{scale}} < P_0$, red $P_0 \leq \frac{p_{sh}}{p_{scale}} < P_{low}$, green $P_{low} \leq \frac{p_{sh}}{p_{scale}} < P_1$, blue $P_1 \leq \frac{p_{sh}}{p_{scale}} < P_{high}$

SURFplus

- SURFplus is an extension of the SURF model that adds a second slower reaction the follows a burn using SURF
  - The fast reaction corresponds to molecular decomposition and leads to intermediate products.
  - The second reaction burns the intermediate products to produce the final products
- The model system is coupled to the SURF model for the fast reactions via a streamwise ODE and is summarized by the reaction progress variable for intermediate and final products (λ) (mass fractions for intermediate and final products) and relative mass fraction of the final products with respect to the intermediate and final products (λ_2).
- The energy deficit compared to the equilibrium mixture is modeled as

$$e_{cc}(\lambda_2) = \left(\left[\frac{1}{1 + (N_{ratio} - 1)\lambda_2} \right]^{1/3} - N_{ratio}^{-1/3} \right) Q$$

- Equation of state evaluations use the energy offset

$$p(V, e, \lambda, \lambda_2) = p(V, e - \lambda e_{cc}(\lambda_2), \lambda)$$

Where $p(V, \cdot, \lambda)$ is the pressure-temperature equilibrium solution for a mixture of reactants and final products

SURFplus: Evolution equations

- The evolution equation for λ_2 is modeled as

$$\frac{Ds_2}{Dt} = \frac{1}{2} \lambda_2 \begin{cases} \frac{h_1 a_2}{h_1 s_2 + (t_1 a_2 - h_1)(h_1^{1/2} - s_2)} & s_2^2 < h_1 \\ a_2/s_2 & h_1 \leq s_2^2 \leq h_2 \\ [2(1 - s_2^2) a_3]^{1/2}/s_2 & h_2 < s_2^2 \end{cases}$$

- $s_2 = \sqrt{\lambda_2}$, $a_2 = \frac{h_2 - h_1}{t_2 - t_1}$, $a_3 = \frac{a_2^2}{2(1 - h_2)}$
- t_1 , t_2 , h_1 , h_2 along with N_{ratio} and Q are parameters of the model
- For PBX-9502 we used the following values

Parameter	Value	Parameter	Value	Parameter	Value
Q	3	t_1	0.005	t_2	0.4
N_{ratio}	50	h_1	0.001	h_2	0.95

- Note the parameters for time are dimensionless and are actually in units of t_{scale} . The units for Q should be in $\frac{p_{scale}}{\frac{gram}{cc}}$. For the units scaling used here of pressure in gigapascals the specific internal energy units would be kilojoules/gram

PBX-9501: Programmed Burn Setup

- The Cyclops I experiment used a PBX-9501 booster to initiate the reaction in the PBX-9502. A detailed high explosive model was not needed for the booster reaction. Since the booster explosive geometry is a simple rectangle the line of sight programmed burn model was sufficient.
- The PBX-9501 burn was started at the location (6,-0.2)
- The CJ reactants detonation speed was $D_{CJ} = 8.8$ km/sec
- The CJ reactants pressure used was $P_{CJ} = 38.6358$ GPa.
- The pseudo reaction time used the dimensionless value of 1.
- In this model, burn is started at location when the spherical wave starting at the initiator location with velocity D_{CJ} reaches that point, at which point the pressure is increased to P_{CJ} and all reactants are converted into products. In this application the energy release due to the reaction was incorporated into the reaction products equation of state.

The Cyclops I Experiment

Experiment Background

- The Cyclops I high explosive experiment was conducted in 2010 at the Los Alamos National Laboratory to observe the behavior of the insensitive high explosive PBX-9502
  - PBX-9502 is a polymer-bonded explosive consisting of 95% by mass of the insensitive explosive TATB (triaminotrinitrobenzene) and 5% by mass of the Kel-F (Polychlorotrifluoroethylene) binder
- References:
  1. Terrones, G., M.W. Burkett, and C.L. Morris, *Burn front and reflected shock wave visualization in an inertially confined detonation of high explosive*. AIP Conference Proceedings, 2012. **1426**(1): p. 239-242.
  2. Hughes, J.M. and G. Terrones, *PAGOSA Simulations for the LANL Blast Tube*, Los Alamos National Laboratory, LA-UR-18-27325. 2018.
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  4. Terrones, G., *Cyclops Proof Shot*, Los Alamos National Laboratory, LA-UR-10-03963. 2010.
  5. Terrones, G., M.W. Burkett, and C. Morris, *Burn Front Data from the Cyclops I Experiment*, LA-UR-11-07121. 2011.
  6. Terrones, G., M.W. Burkett, and C. Morris, *Burn Front and Reflected Shock Wave Visualization in an Inertially Confined Detonation of High Explosive*, Los Alamos National Laboratory, LA-UR 11-03382. 2011.
  7. Terrones, G., et al., *Cyclops Experiment*, Los Alamos National Laboratory, LA-UR-10-04469. 2010.

Experimental Device

- The device consisted of a steel cylinder containing PBX 9502 with an inner shell of tin in the form of an ellipse whose major axis is rotated relative to the detonator.
- A photograph of the apparatus taken from reference 1 is shown on the right.
- The experiment was diagnosed with a set of eight Photon-Doppler-Velocimetry (PDV) probes on the outside of the device and proton radiography images of the explosion at one microsecond intervals.
- A schematic of the device showing dimensions is shown on the right.
- The PBX-9502 was ignited using a line wave generator (LWG) to ignite a PBX-9501 booster that penetrates the steel shell.

Simulation Setup

Background

- This experiment was simulated using the Los Alamos Eulerian Applications Code xRage
  - xRage is a fixed grid Eulerian code with adaptive cell-by-cell mesh refinement
- The flow model is the multi-material inviscid Euler equations
  - Mixed cells are treated using the Amagat material separated equation of state model with pressure-temperature equilibrium
- The high explosives are modeled using the SURFplus reactive burn models coupled to the xRage Eulerian solver
  1. Menikoff, R. and M.S. Shaw. *Reactive burn models and ignition & growth concept*. in *EPJ Web Confs.* 10. 2010. EDP Sciences.
  2. Shaw, M.S. and R. Menikoff. *A reactive burn model for shock initiation in a PBX: scaling and separability based on the hot spot concept*. in *Fourteenth International Symposium on Detonation*. 2010. Coeur d'Alene, Idaho, USA: US office of naval research.
  3. Menikoff, R. and M.S. Shaw, *The SURF model and the curvature effect for PBX 9502*. *Combustion Theory and Modelling*, 2012. **16**(6): p. 1140-1169.
  4. Menikoff, R., *Shock Detector for SURF Model*, Los Alamos National Laboratory, LA-UR-16-20116. 2016.
  5. Menikoff, R., *SURFplus Model Calibration for PBX 9502*, Los Alamos National Laboratory, LA-UR-17-31015. 2017.

Simulation Setup

- The computational domain extends from $-7.5 \text{ cm} \leq x \leq 17.5 \text{ cm}$ and $-7.5 \text{ cm} \leq y \leq 7.5 \text{ cm}$ in standard Cartesian geometry.
- The base computational mesh used square grid blocks of size 200 microns = .02 cm.
- The AMR specification for the various materials are described in the following table

PBX 9502 Burn Zone Size	PBX 9501 Burn Zone Size	Air	PBX 9501 reactants and products	PBX 9502 reactants and products	Sylgard	Stainless Steel SS-304L	Tin
200	200	200	200	200	100	100	100
100	100	100	100	100	100	100	100
50	50	100	50	50	50	50	50
25	50	100	50	25	50	50	50
12.5	200	200	200	12.5	200	25	25
6.25	200	200	200	12.5	200	25	25

- The experiment used Nusil gel 8150 to bind the PBX-9502 to the metal shells, but due to lack of equation of state data for this material we substituted the Nusil gel with the Sesame material for Sylgard.
  - Both materials are silicon based elastomers and should have similar hydrodynamic properties.

Initial Conditions

- The figure shows the initial geometry used for the Cyclops I setup

Initial Conditions: Jet Confiner

- The main difference in the computational setup and the experiment was the addition of a block of plastic around the PBX-9501 booster.
- This block was needed to suppress mixing between the ejected PBX-9501 products and the background air. Without this box xRage gets a time step crash due to mixing between these two materials.
- The box has no effect on the propagation of the PBX-9502 burn front in the interior of the device. It just helps avoid a time step crash unrelated to the HE burn model.
- A illustration of this jet is shown on the right.
  - Note that for a Lagrangian simulation this jet would be a source of grid tangling.

Initial Conditions: Flow Cauchy Data

- The table below summarizes the initial conditions used for these simulations. All materials are initially at rest.

Material	Pressure (Mbar)	Temperature (K)	Density (grams/cc)	Specific Internal Energy (tera erg/gram)
Air	1.0×10^{-6}	296.15	0.001	2.5×10^{-3}
SS-304L Steel	1.0×10^{-6}	296.15	7.89	8.48×10^{-5}
Tin	1.0×10^{-6}	296.15	7.27	2.53×10^{-5}
Sylgard	1.0×10^{-6}	296.15	1.04	-2.8×10^{-5}
PBX 9501 reactants	1.0×10^{-6}	296.15	1.894	-3.61×10^{-5}
PBX 9502 reactants	1.0×10^{-6}	296.15	1.84	-4.43×10^{-5}

- The PBX-9501 was initiated using a program burn for a point on the right hand side of the booster 2 mm below the x-axis.

Hydrodynamic Equation of State Models

- The background material for the simulation is air modeled as a perfect gas with Grüneisen coefficient $\Gamma = \gamma - 1 = 0.4$ and a specific heat at constant volume of $C_V = 8.4417 \times 10^{-6} \frac{\text{Tergs}}{\text{gram K}}$.
- The high explosive reactants and products used Sesame equations of state.

Material	Sesame ID	Material	Sesame ID	Material	Sesame ID
PBX 9501 Reactants	950104	PBX 9502 Reactants	950202	Sylgard	97932
PBX 9501 Products	8211	PBX 9502 Products	950211		

- The metal shells were modeled using the Steinberg-Mie-Grüneisen equation of state with constant specific heats at constant volume

$$P - P_r(V) = \frac{\Gamma(V)}{V} (e - e_r(V)) = \frac{\Gamma(V)}{V} C_V (T - T_r(V))$$

$$C_V \left\{ T_r'(V) + \frac{\Gamma(V)}{V} T_r(V) \right\} = e_r(V) + P_r'(V)$$

- For compression the reference pressure and specific volume assume a linear relation between the shock velocity (U_S) and particle velocity behind the shock (U_P) at constant compression $U_S = c_0 + sU_P$ where s is a quadratic function of the compression $(V_0 - V)/V_0$
- For expansion the stiff gamma law equation of state is used.

Steinberg Equation of State Parameters

- We used the equation of state parameters for SS-304L stainless steel and tin taken from the report
  - Steinberg, D.J., *Equation of State and Strength Properties of Selected Materials*, Lawrence Livermore National Laboratory, UCRL-MA-106439-rev. 1996.
- The table below summarized the values for the Steinberg-Mie-Grüneisen equation of state used for this study.

Material	Steel (SS-304L)	Tin
Reference density (ρ_0) grams/cc	7.9	7.287
Grüneisen exponent at reference density (Γ_0)	1.93	2.27
Grüneisen exponent at infinite compression (b)	0.5	0.54
Reference sound speed (c_0) cm/ μ sec	0.457	0.259
S_1	1.49	1.49
S_2	0	0
S_2	0	0
Specific heat at constant volume (C_V) $\frac{\text{Teraerg}}{\text{gram}} / ^\circ K$	1.2417×10^{-4}	3.051×10^{-5}

Material Strength Models

- Both the steel and tin shells that bound the PBX-9502 were modeled using the Steinberg-Cochran Guinan hypoelastic-plastic flow model.
  - Steinberg, D., S. Cochran, and M. Guinan, *A Constitutive Model for Metals Applicable at High Strain-Rate*. J. Appl. Phys., 1980. **51**: p. 1498-1504.
- The material parameters used are summarized in the table below.

Material	Stainless Steel SS-304L	Tin
Shear Modulus, (G_0) Mbar	0.770	0.179
Yield Strength, (Y_0) Mbar	3.4×10^{-3}	1.6×10^{-3}
Pressure dependence for the shear modulus (A) 1/Mbar	2.26	8.66
Temperature dependence for the shear modulus (B) 1/°K	4.55×10^{-4}	2.12×10^{-3}
Work hardening parameter (β) Mbar	43.0	2000.0
Initial plastic strain	0	0
Work hardening maximum (Y_{max}^*) Mbar	2.5×10^{-3}	2.2×10^{-3}
Coefficient of volume dependence of the Grüneisen exponent	$\Gamma_0 - b$	$\Gamma_0 - b$
Melt (T_{mo}) °K	2380	656.6

Photon-Doppler-Velocimetry Validation

PDV Validation

- When the burn front shock wave interacts with the bounding metal shells, transmitted waves are created which reverberate inside the shells and transmit waves into the bounding materials. When this lead burn front shock passes near a PDV location in the steel shell these waves propagate through the shell and are picked up by the PDV probes as motion of the outer steel shell.
- The arrival times for the burn fronts at the PDV locations were tracked using Lagrangian tracers
  - Currently xRage does not support true PDV probes in Cartesian geometry
  - The main difference between Lagrangian tracers and PDV probe tracers is that PDV probes are constrained to only move in the direction of the PDV probe beam.
  - This difference means that the Lagrangian probes will move away from the probe beam with time resulting in an effectively higher velocity since they stay closer to the lead burn wave than a true PDV probe.
  - In our case the Lagrangian tracers are sufficient to get the first arrival time at the probe location.

PDV Probe Locations

Convergence Results for Shock Arrival Times

- We performed a convergence analysis for the time of first arrival of the burn front at the eight PDV probe locations.
- The velocity at the Lagrangian Tracers was extracted from the text file xRage prints for the tracer data and processed using a MATLAB script.
- The experiment did not record a starting time. This value was estimated by fitting the experimental data to align with the first PDV probe computed arrival.
- A linear regression analysis shows that the first arrival times at the probes converge to experiment at approximately first order.

Arrival Time Convergence

- At low resolutions all of the probes show a lag in the first arrival time of the burn front
- At higher resolutions this lag largely disappears
  - By the 6.5 micron case the arrival times are very close to the experimental values
- The arrival time for the experimental data was set by locating the first sharp rise in the PDV data
- Computational arrival times were found by locating the time of the pressure maximum at the Lagrangian tracers.
- Probe 5 is somewhat different from the other probes since at the time of first arrival it is experiencing two burn front accelerations from either side of the device.
  - The first jump for the experiment line up will with the higher resolution data
  - The second jump comes about .3 microseconds after the first jump and is not readily apparent in the computations.

PDV Probes 1-3 Arrival Times

**xRage SURF+ versus experimental PDV velocities
Probe 1**

**xRage SURF+ versus experimental PDV velocities
Probe 2**

**xRage SURF+ versus experimental PDV velocities
Probe 3**

PDV Probes 4-6 Arrival Times

**xRage SURF+ versus experimental PDV velocities
Probe 4**

**xRage SURF+ versus experimental PDV velocities
Probe 5**

**xRage SURF+ versus experimental PDV velocities
Probe 6**

PDV Probes 7 and 8 Arrival Times

**xRage SURF+ versus experimental PDV velocities
Probe 7**

**xRage SURF+ versus experimental PDV velocities
Probe 8**

Verification Results

- We use the 6.5 micron as a pseudo fiducial solution and compute the rates of convergence of the coarser resolutions to the fiducial for the finest arrival time (peak pressure for the probe data)
- The arrival times show first order convergence
- The velocity at time of first arrival is nearly constant and does not show any significant convergence behavior
- Pressure shows a considerable spread at low resolution and appears to be nearly constant at higher resolutions

Proton Radiography Validation

Proton Radiography Images

- The Cyclops I experiment was imaged using proton radiography with data in the form of an audio video interleave (AVI) movie generated from the PRAD photographs.
- The individual frames of this movie were extracted using MATLAB image processing tools in the form of nineteen 1161×1161 pixel raster files.
- These raster files were used to create EnightGold format files that could be overlaid with the computed solutions.
  - Enight provided a number of useful functions that included
    - Panning and zooming
    - Modification of color maps
    - Ability to easily move forward on backward in time over the images
    - Adding annotations
- It was determined that the images were taken at one microsecond intervals starting four microseconds after booster ignition.

One Movie Shows it All

What We See

- The movie on the preceding slide shows two series of images, the first for the computed density field and the second for the computed gradient of density field overlaid on the PRAD photographs.
- Each series shows the results for the computed solution at a series of resolutions.
- As the resolution increases (finer mesh at the burn front) the velocity of the front increases and converges toward the experimental interface.
- We clearly see the reverberated waves in metal shells that impact the PDV measurements.
- The biggest difference is in the position and shape of the metal shells
  - Not directly relevant for the HE burn front validation as the difference occur downstream from the burn front
- At later times the steel shell is deflected outward compared to experiment
- The large dent in the tin interface seen in the experiment is noticeably smaller in the computation
- These differences in the metal shell behaviors suggest the Steinberg-Guinan strength model is not completely consistent with the real behavior of the metal shells
  - Other models might yield improvements

Quantitative Convergence Validations

- Quantitative metrics for the convergence of the isochrone burn fronts required fitting the computation and experiment fronts
  - The Enight spline tool proved very useful in fitting the computations.
  - The SURF burn model detects the high explosive ignition using the value of the Hugoniot function. This field is printed in the xRage restart dumps and could be used to fit a spline curve to the lead front.
- Isochrone spline fits were computed for each of the six resolution levels and thirty time frames using the Enight spline tool.
- These fits were further smoothed using smoothing spline tools available from the MATLAB curve fitting package.

Experimental Isochrone Fits

- Fitting spline curves to the experimental PRAD images was complicated due to the low resolution of the images.
- Three curves were fit by hand corresponding the leading edge of the burn profile, the middle region, and the trailing edge.
- The difference between the leading and trailing edges gives a rough estimate of the uncertainty in the burn front location.
- The leading edge position is most comparable to the computational fits.

Qualitative Convergence (eye-ball norm)

- Each of the isochrones are labeled by the time in microseconds when the PRAD image was taken. Each time yields two isochrones, one for the upper section of the device (labeled U) and one for the lower section (labeled L).
- These images occur at times ranging from four to eighteen microseconds.
  - Beyond eighteen microseconds the upper and lower burn fronts have collided.
- The figure shows the computed and experimental isochrones superimposed.
- With increased refinement the computed values converge towards experiment

Blow-up of Isochrones at 16 microseconds

- The picture on the previous slide is a bit difficult to see.
- Below are blow-ups of the 16 microsecond images.

- By the 6.25 micro resolution the computed and picked isochrones agree closely in position
- The resolution of the PRAD photographs was not sufficient to see the curvature at the inner edge of the channel.

Convergence Rates for Isochrones

- For each of the isochrones from four to eighteen microseconds we computed the convergence rate to the experimental data using log-linear regression.
- The convergence was computed at a common arc length along each isochrone.

Integrated Convergence Rates

- If we integrate the convergence rates along each isochrone we get a picture of an average convergence rate.
- The figure shows convergence of the averaged rates of about first order on the 16 microsecond isochrone.
  - The metric is the convergence rate of the integrated difference between the computed and picked isochrone positions as a function of arc length.
- The 200 micron case is an outlier. For resolutions finer than 200 the actual rate will be higher
- We see a slight glitch at 6.25 micron resolution on the lower isochrone. At this point the grid size is comparable to the grain size so the continuum assumption may be becoming invalid.
- This feature may also be related to the somewhat subjective fit to the PRAD data.
- Similar rates are seen on all of the isochrones.

Verification Rates

- The relatively poor resolution of the experimental PRAD images makes detailed comparisons subject to a substantial “human” error in picking out the locations of the PRAD measured burn fronts.
- We also computed solution verification rates based on the 6.25 micron resolution case as a fiducial.
- In this case we get approximate first order convergence towards the fiducial.

Upper 16 microsecond Isochron
Simulation Convergence Rate
Mean = 1.16045

Lower 16 microsecond Isochron
Simulation Convergence Rate
Mean = 1.03171

Integrated Verification Rates

- As with the experimental rates we computed the integrated convergence rates.
- As before this is convergence rate of the integral of the difference between the isochrones as a function of arc length.
- We note the the glitch at the finest resolution seen in the experimental comparison is not apparent.
  - Of course the glitch occurred at the finest resolution, which is now take as the fiducial, so the absence of the glitch is perhaps not surprising.
- As before the 200 micron case is an outlier

Convergence Rate Summary

- Lack of space and time prevent showing graphs of the rates for all of the isochrones. The table below gives a summary for all of the isochrones

Isochrone Arrival Time microseconds	Lower Isochrone Mean Convergence Rate Computation to Experiment	Upper Isochrone Mean Convergence Rate Computation to Experiment	Lower Isochrone Mean Convergence Rate Computation to Fiducial	Upper Isochrone Mean Convergence Rate Computation to Fiducial
4	0.707116	0.186394	1.10166	1.78911
5	0.744946	0.287773	1.15774	1.39983
6	0.950369	0.34758	1.19751	1.49275
7	0.37414	0.380441	1.19203	1.34514
8	0.393144	0.406448	1.13889	1.28526
9	0.801305	0.402676	1.15045	1.27982
10	0.654035	0.498127	1.12111	1.15437
11	0.548552	0.511603	1.13857	1.25483
12	0.566443	0.435021	1.06179	1.16364
13	0.650162	0.548418	1.1099	1.26979
14	0.84343	0.50915	1.05048	1.19117
15	0.770116	0.507175	1.02866	1.2005
16	1.04506	0.738567	1.0429	1.16092
17	0.652512	0.629139	1.00663	1.11089
18	0.56787	0.753479	0.960375	1.04437

Average Rate Over All Isochrones

- As a final convergence metric we computed the average over all isochrones for the positional convergence, both to experiment and to the 6.25 micron fiducial.
- Convergence towards experiment is about $\frac{1}{2}$ order and about first order towards the fiducial

Burn Front Curvature

- One of the features of the SURFplus model is to incorporate the geometric source terms corresponding to burn front curvature into the SURFplus fitting forms.
- We test the success of these fits by examining the burn front curvature compared both the experiment and the simulation fiducial.
- The two figures show the gradient of density superimposed over the PRAD images for the 50 micron and 6.25 micron cases.

Experimental Curvature Comparison

- The somewhat “ad hoc” fitting for the PRAD isochrones is subject to considerable variation in the fitted front curvature
- The figures show the computed verses experiment fitted front curvatures.
- The computations are indicating a convergence towards the finest resolution, but the experiment fits are all over the place

Curvature Verification

- The noisy resolution at the fine scale needed to fit the experiment led us to focus instead on a verification of the curvature convergence rather than an explicit validation to the experiment.
- As before we use the example of the 16 microsecond isochrones compared to the 6.25 fiducial.
- Comparing the integrated difference of the curvatures for each resolution to the 6.25 micron fiducial we see about $\frac{3}{4}$ accurate convergence behavior
- The average over all isochrones shows about a half order accurate convergence

Sobolev Convergence

- As a final converge test we compute the $W^{2,1}$ norm for the difference of the solutions compared to the 6.25 micron fiducial, where the norm for the Sobolev space space $W^{k,p}$ is defined as

$$\|f\|_{k,p} = \left(\sum_{i=1}^k \|f^{(i)}\|_p^p \right)^{1/p} = \left(\sum_{i=1}^k \int |f^{(i)}(t)|^p dt \right)^{1/p}$$

- The figures indicate that for this norm we are getting close to first order converged in the combined position and shape for the burn front geometry compared to the 6.25 micron fiducial
  - We note that this norm is dominated by the position differences

Conclusions

- We discussed a variety of convergence metrics for the validation of the xRage simulations of the Cyclops I experiment based on two diagnostics, photon-Doppler-velocimetry and proton-radiography images.
- The simulations show the expected convergence properties under mesh refinement of the reaction front resolution from 200 down to 6.25 microns.
- The PDV probe comparisons agreed with experiment for the time of arrival of the high explosive generated shock wave at the outer edge of the steel shell to within a couple of percent and the finer resolutions agreed with experiment at the 1% or better level.
- The average for the spline fit isochrones showed convergence to the experimental fit isochrones to better than a half order of accuracy and the computed positions agreed with experiment to better than 5% for resolutions less than 50 microns and no worse than about 10% for all resolutions. At the finest level of refinement, the agreement with the isochrone positions was under 1%.

Conclusions

- We also discussed verification metrics to illustrate that self-consistency of the xRage code and its implementation of the SURFplus model under mesh refinement.
- These metrics show that SURFplus combined with the xRage hydrodynamics method achieve on average a better than first order convergence to the finest grid simulation taken as the fiducial.
- Since these positions are all related to the lead shock front, first order convergence is the best that could be expected for a conservative Godunov algorithm.
- Based on the above metrics both in terms of agreement with experiment and solution verification we can have good confidence with the simulation results using the SURFplus high explosive model for all resolutions finer than 50 microns (about two mesh zones in the reaction profile) and that even at coarser resolutions the calculations agree with experiment to within 10%.