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Title: Comparison Between Surf and Multi-Shock Forest Fire High Explosive Burn Models

Author(s): Greenfield, Nicholas Alexander

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Nick Greenfield

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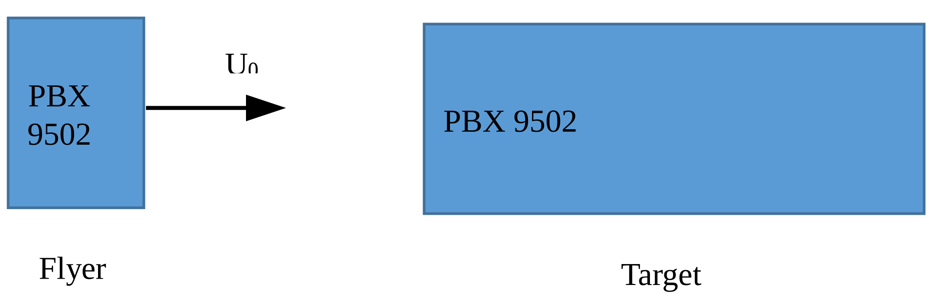
PAGOSA[1] has several different burn models used to model high explosive detonation. Two of these, Multi-Shock Forest Fire and Surf, are capable of modeling shock initiation. Accurately calculating shock initiation of a high explosive is important because it is a mechanism for detonation in many accident scenarios (i.e. fragment impact). Comparing the models to pop-plot data give confidence that the models are accurately calculating detonation or lack thereof. To compare the performance of these models, pop-plots[2] were created from simulations where one two cm block of PBX 9502 collides with another block of PBX 9502. The simulation was run in 3D but only the minimum number of cells, which is three, were used in the x and y direction (an example PAGOSA input file is included in the appendix). These were also compared to the experimental pop-plot data[3]. The following equation fits that experimental data:

Eq 1: $\ln(x) = -6.3471 - 23471 - 2.9175 \ln(P)$

Where x is run distance and P is initial pressure.



Simulations were run at five different initial pressures (0.08, 0.10, 0.12, 0.15, and 0.2 Mbar) and with five different mesh sizes (300, 400, 500, 600, and 700 microns). The different initial pressures were achieved by changing the velocity of the flyer. The below equation[4] relates initial pressure to the flyer's velocity. Tracers were placed every 500 microns to record pressure data.

Eq 2: $$U_0=\frac{c_0}{s}\left(\sqrt{1+\frac{4sP_0}{\rho_0 c_0^2}}-1\right)$$

For PBX 9502[5]:
c_0 = 0.240 cm/ μs
ρ_0 = 1.894 g/cm^3
s = 2.050

The run distance for each simulation was determined two different ways. The first method was to find the first tracer that reached 0.285 Mbar. This threshold is 95% of the detonation pressure for PBX 9502. The second method was to look at the derivative of the plot of each tracer's peak pressure. Detonation occurs when the peak pressure starts to level off, so when the derivative of each peak tracer pressure first goes to zero detonation is reached (example: Figure 1).

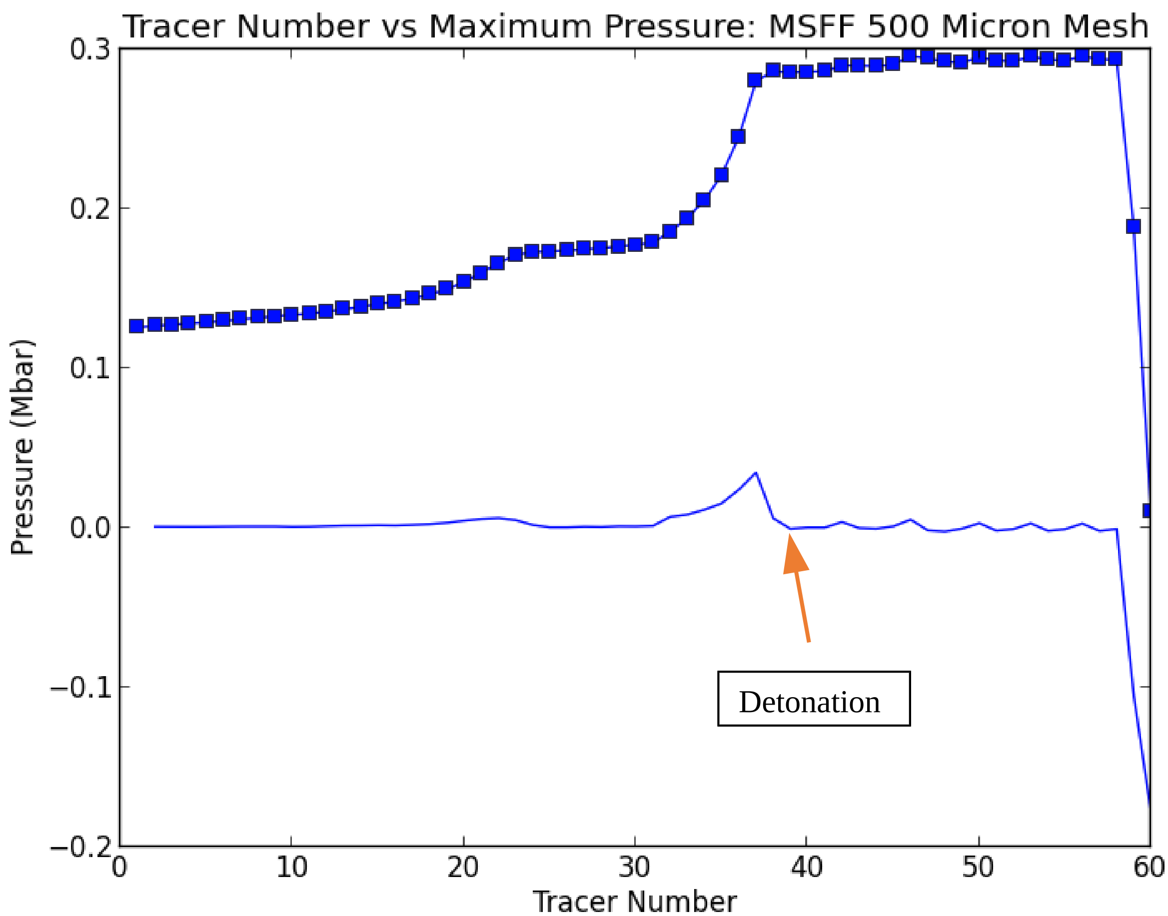


Figure 1: Upper curve shows the maximum pressure for each tracer. Lower curve is the derivative of the upper curve.

Below are the pop-plots for both Surf and Multi-Shock Forest Fire (Figures 2, 3, 4, and 5):

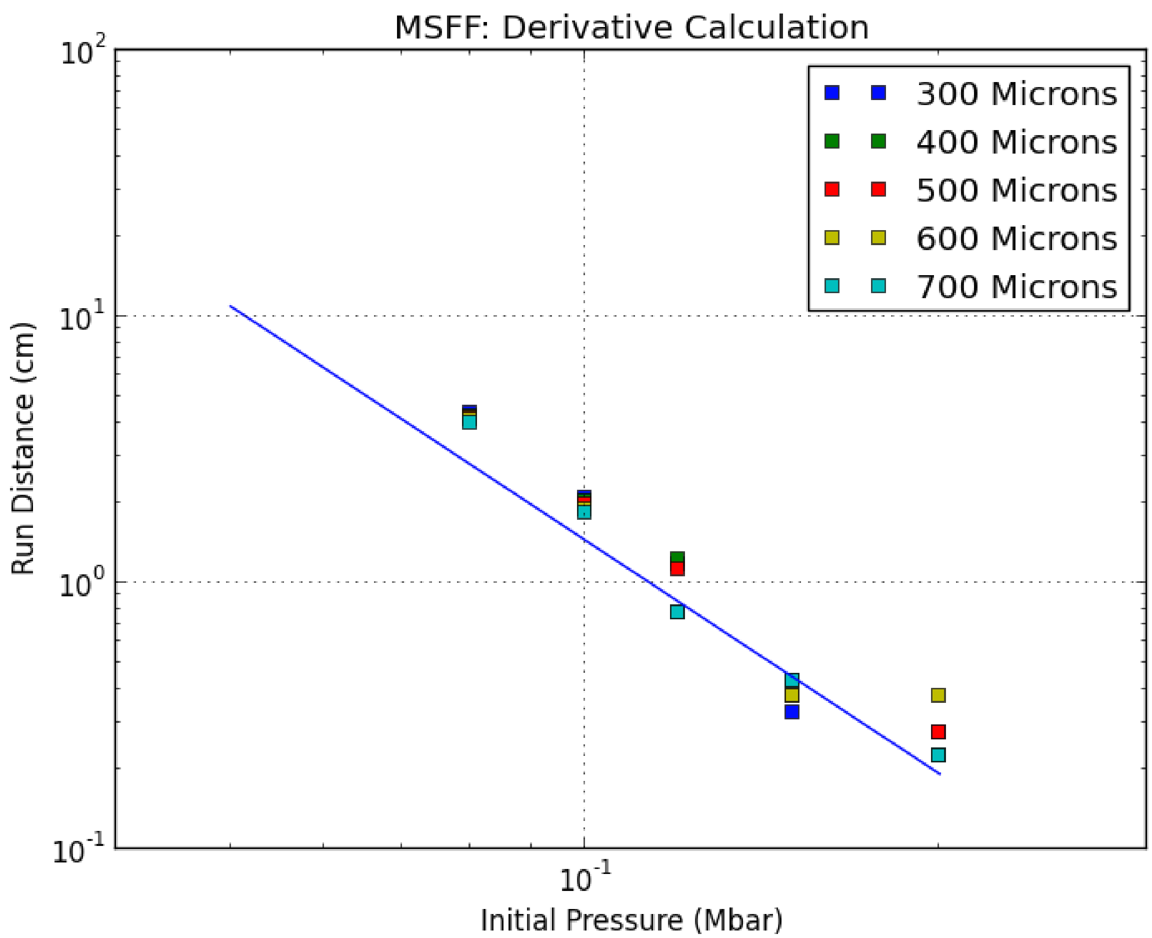


Figure 2: Pop-plot of simulation using MSFF for five different mesh sizes. Run distance calculated with the derivative method. Line is the experimental results from Eq 1.

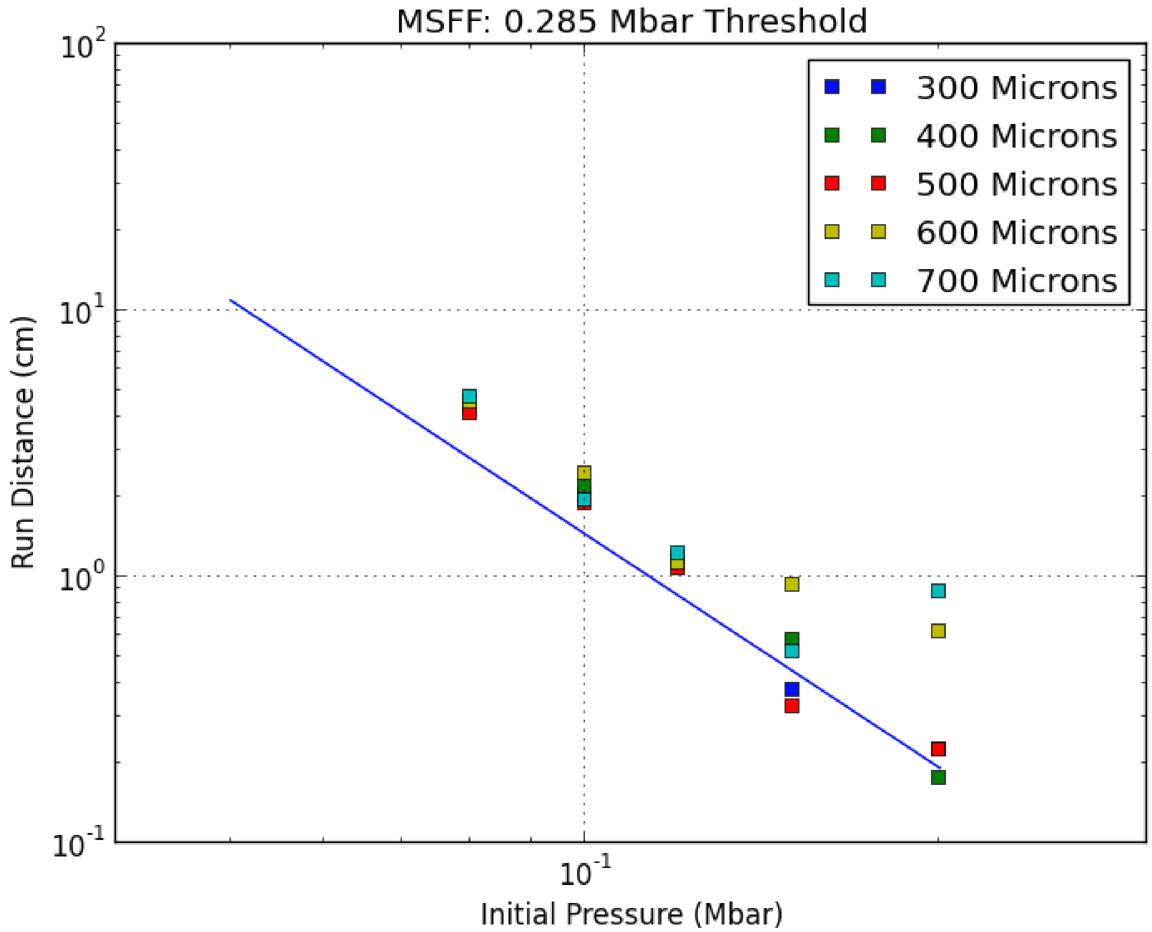
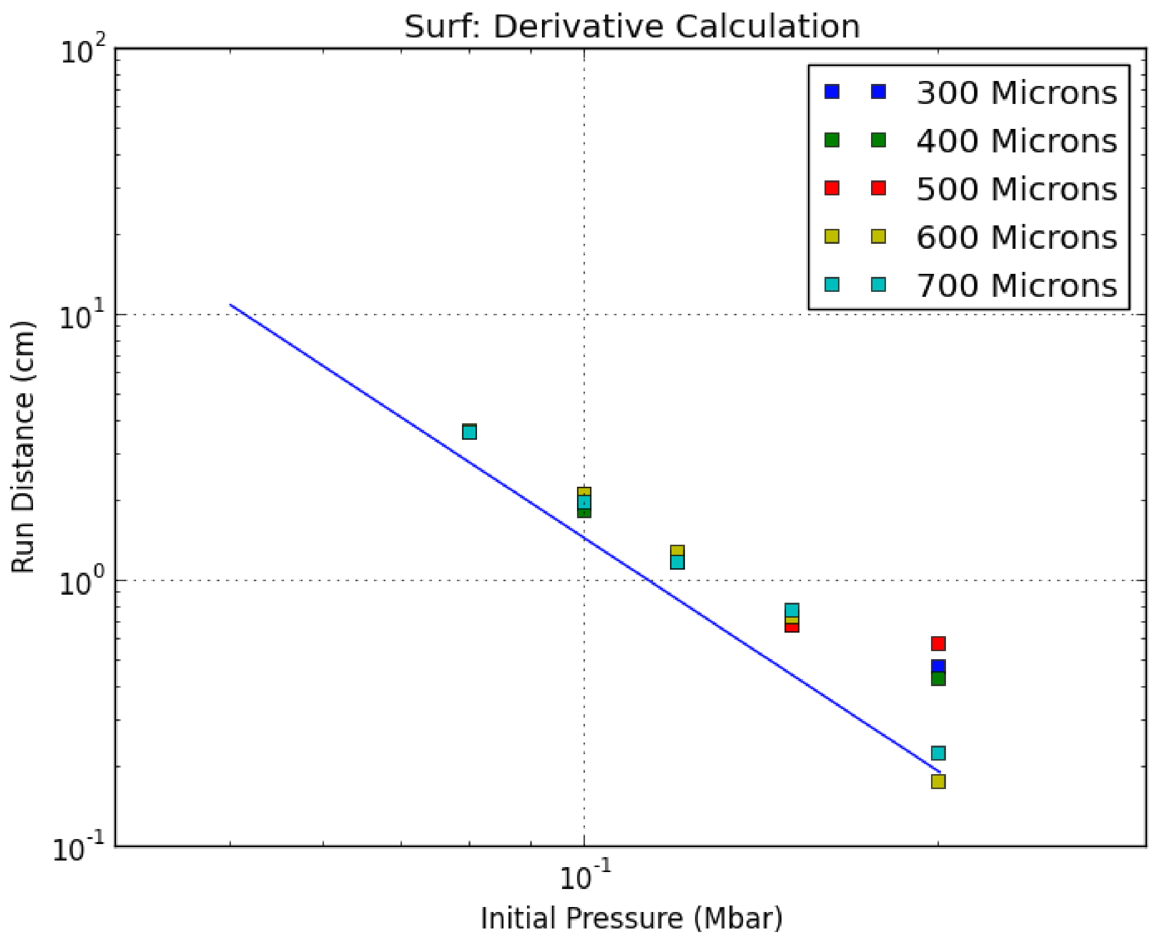


Figure 3: Pop-plot of simulation using MSFF for five different mesh sizes. Run distance calculated with the threshold method. Line is the experimental results from Eq 1.



Surf: Derivative Calculation
300 Microns
400 Microns
500 Microns
600 Microns
700 Microns
Run Distance (cm)
Initial Pressure (Mbar)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-1}

Figure 4: Pop-plot of simulation using Surf for five different mesh sizes. Run distance calculated with the derivative method. Line is the experimental results from Eq 1.

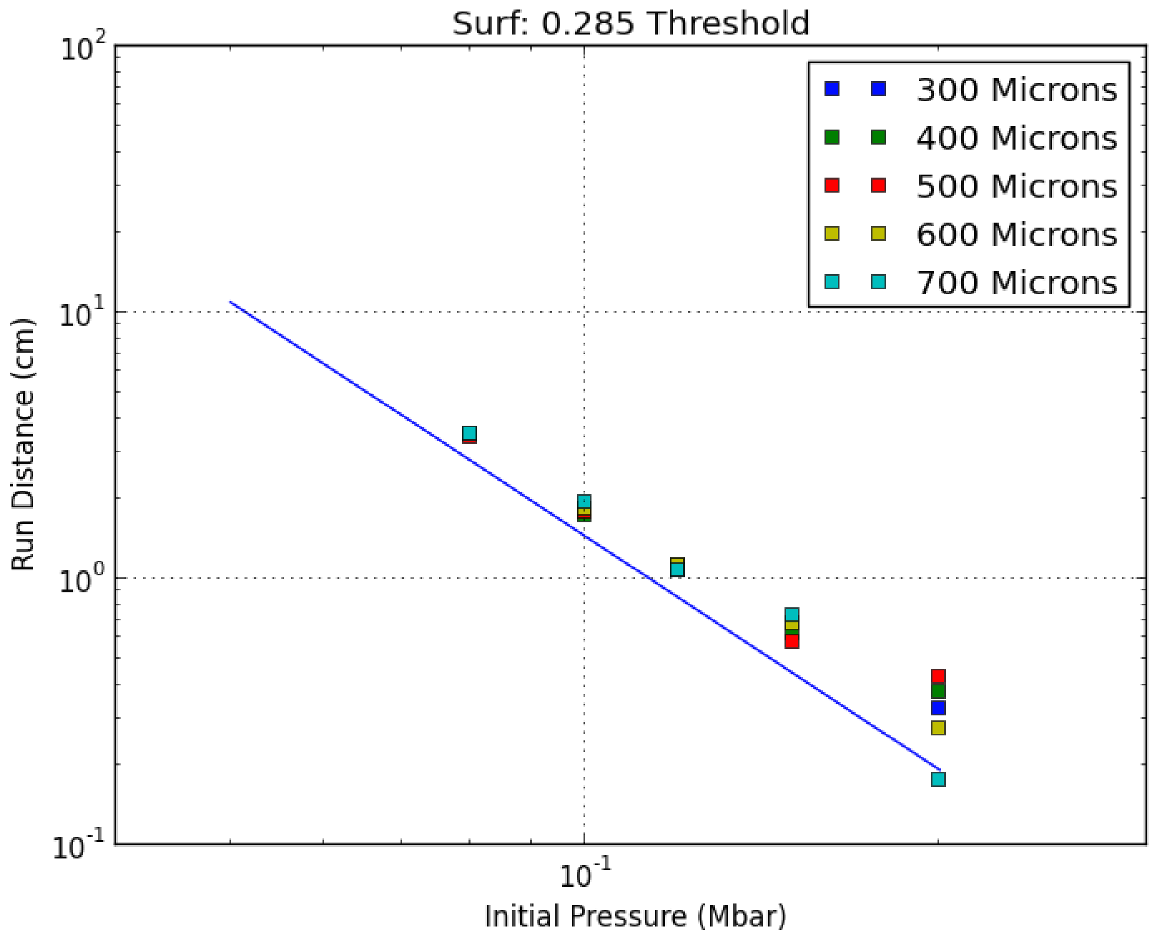


Figure 5: Pop-plot of simulation using Surf for five different mesh sizes. Run distance calculated with the Threshold. Line is the experimental results from Eq 1.

Looking at Figures 2 and 3, it's apparent that using the derivative method to calculate run distance provides more accurate representation of the detonation for the multi-shock forest fire model. The difference in the two methods to calculate run distance for the surf model is minimal, but it appears that using the 0.285 Mbar threshold is more accurate (Figures 4 and 5). The reason the threshold values were less accurate than the values obtained from the derivative method for the multi-shock forest fire model was that the pressure would level off, and thus detonate, a little below the threshold value. The pressure would not reach 0.285 Mbar until several tracers after the actual detonation (Figure 6). This behavior was most notable for the larger mesh sizes. The surf model did not exhibit this behavior (Figure 7), which is why both methods for calculating run distance yield similar results.

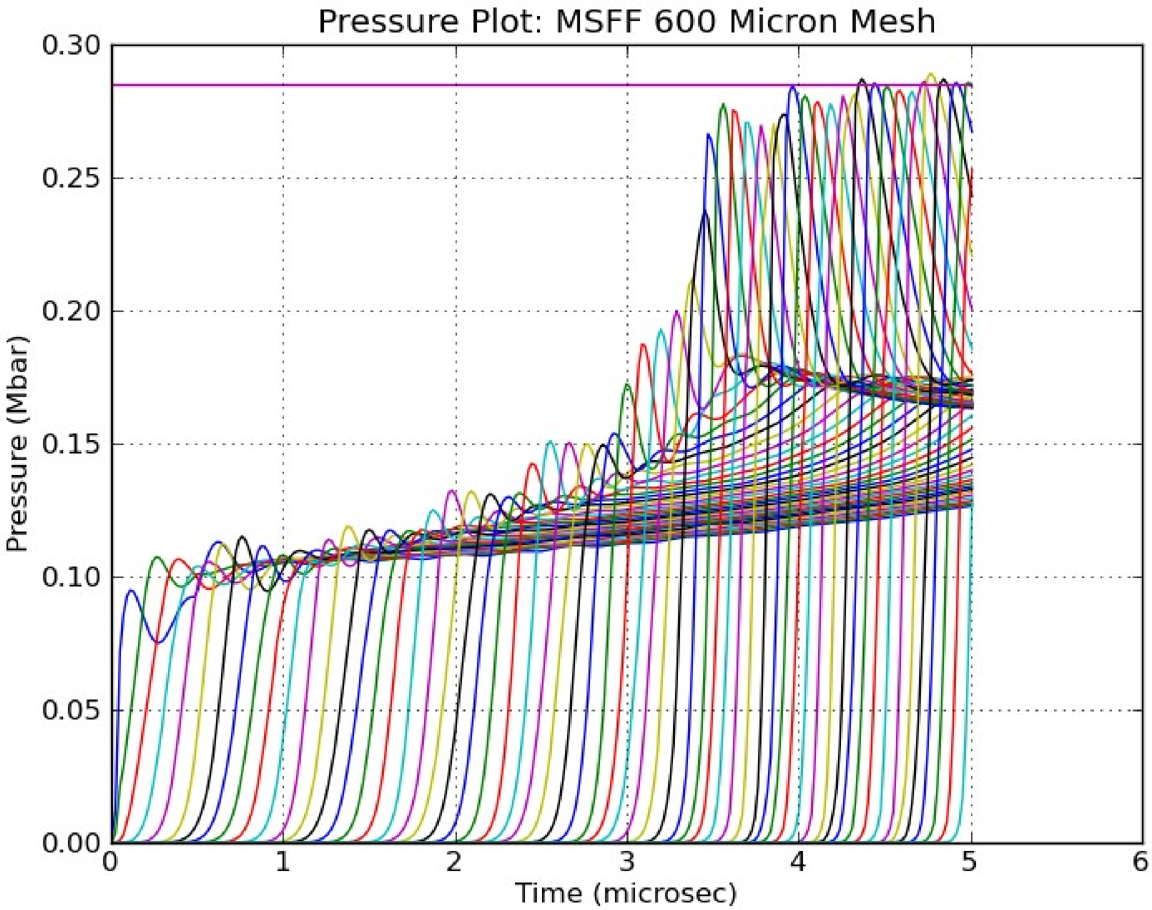


Figure 6: Pressure plot for MSFF with 600 micron mesh. Horizontal line indicates 0.285 Mbar.

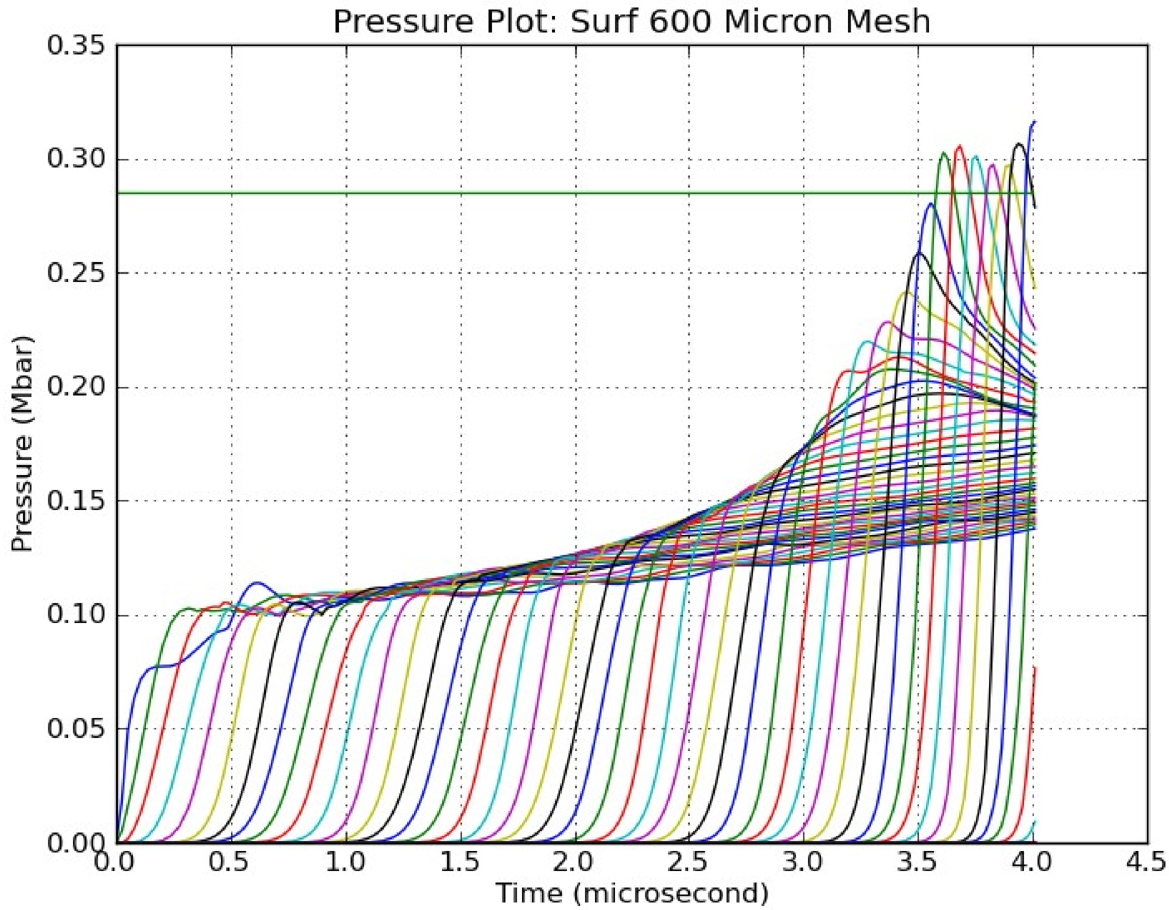


Figure 7: Pressure plot for Surf model with 600 micron mesh. Horizontal line indicates 0.285 Mbar.

Surprisingly, mesh size did not have a consistent effect on the results of this simulation. It was expected that the larger mesh sizes would give poor results. However, the 700 micron mesh actually had the best representation of the detonation when using the Multi-Shock Forest Fire model with the derivative method (Figure 2). The largest initial pressure for the Multi-Shock Forest Fire with the threshold method was the only data point where the 700 and 600 micron mesh was significantly less accurate than the smaller mesh sizes (Figure 3). The initial pressure, rather than mesh size, seemed to control the size of the error. For all the simulations, the larger initial pressures had the largest error. It should be noted that this was a very simple simulation so accuracy of the larger mesh sizes will probably not hold up in more complicated problems. While agreement to experimental data is sensitive to the method used to diagnose detonation, the calculations show reasonable agreement to experimental pop-plot data, at the mesh sizes studied. These results give confidence that Surf and Multi-Shock Forest Fire calculate shock initiation of PBX 9502 with acceptable accuracy.

Acknowledgments

The Author would like to acknowledge his mentor, Ian Fleming, for assigning this task and Erik Shores for helpful discussion and comments.

References

[1]W. Weseloh, S. Clancy, J. Painter, PAGOSA Physics Manual, LA-14425-M, Los Alamos National Laboratory (August 2010).

[2]Terry R. Gibbs and Alphonse Popolato, Editors, LASL Explosive Property Data (University of California Press, Berkeley, 1980).

[3]Charles Madar, 1998, **Numerical Modeling of Explosives and Propellants**, Second edition, CRC Press,
Boca Raton, CD-ROM (drive:/run/fire.out/9502.OUT).

[4]Paul W. Cooper, 1996, **Explosives Engineering**, Wiley-VCH, New York, pages 203-207 and of
particular interest are equations 18.1 and 18.2.

[5]Ian, Fleming. Personal Communication, June 2017.

Appendix

Example input file:

```
PBX 9502 Impact, Surf, 0.10 Mbar, 500 Micron Mesh
 &mesh
  ncellx =     3,
  coordx =  -0.075, 0.075,
  ratiox =       1.0,
  ncelly =        3,
  coordy = -0.075, 0.075,
  ratioy =       1.0,
  ncellz = 50, 100,
  coordz = -2.5, 0, 5.0
  ratioz = 1, 1,
  npes_x = 1,
  npes_y = 1,
  npes_z = 2 /

 &options
  dt0           = 0.025,
  multidiv_type = 'uniform',
  clean         = false,
  id_geom       = 3,
  ibc           = 0,0,0,0,1,1 /

 &outputs
   t          = 0.0, 4.0,
  dt          = 0.1
  dump_freq   = 5,
  short_freq  = 5,
  tracer_freq = -1,
  tracer_var  = 'bfm',
  tracer_mat  = 1,
  gd_freq     = 5,
  gd_var      = 'd', 'p', 'u', 'v', 'w', 'bfm',
  gd_mat      =  0,  0,   0,   0,   0,    1,
  es_var      = 'd', 'p','uvw', 'bfm',
  es_mat      =  0,   0,   0,     1,
  es_last     = 9, /

 &mats
  material = 1,
  priority = 1,
  matname = '9502',
  d0 = 1.895,
  e0 = 0.0,
```

```
 clean_df = 0.05,
 pmin = 0.0,
  eosform  = 'he-jwl',
  eoscon   = 0.297,       1.81,    0.00000,
            0.89380000,       0.000000000,    3.40000000,
            0.38755650,       -15.63680478,   -1.69414807,
            30.0251610,       21.50000000,
            0.59440730,       0.000050000,
            13.4540000,       0.672700000,    0.013430000,
            11.7180000,       4.158000000,    0.500000000,
            0.03650790,       0.239005740,    3202.000000,
            5.00000000,       0.000100000,
            15.0000000,       10.00000000,
 burnform = 'surf',
 burncon  = 0.01, 0.99, 0.055, 0.24, 6.0,
           43298.11835590, -35356.9929246, 11721.06027920,
           -2015.70898175, 216.2064452280, -12.3288500067,
            1.0, 0.5,
           -3.35, 0.30, 2.0, 20.0, 2.0, 5.0, 0.0,

 detvel = 0.762,
 strform  = 'none',
 strform  = 'ep',
 y0       =  0.0005,
 g0       =  0.03 /

&mats
 material = 2,
 matname = 'void',
 priority = 2,
 eosform = 'void',
 matbak = 2 /

&mats
 material = 3,
 matname = 'Striker',
 priority = 3,
 d0 = 1.894,
 e0 = 0,
 pmin = 0,
 eosform = 'usup',
 eoscon = .24, 2.05, 1.5, 0,
 strform = 'none' /

&gen
 coarse_particles = 8,
 fine_particles = 16,
 start_mode = 1,
```

```
 interactive = false,
 restart_dump = true /

&body
 material_number    = 1,
 surface_name       = 'plane',
 axis               = 'z',
 fill               = '+',
 trans =  0.0, 0.0, 0.0,
 rot   =  0.0, 0.0, 0.0,
 angle =  0.0, 0.0, 0.0, /

&body
 material_number    = 3,
 surface_name       = 'plane',    'plane',
 axis               = 'z',         'z',
 fill               = '-',         '+',
 trans               =  0.0, 0.0, 0.0,
                       0.0, 0.0, -2.0,
 rot                 =  0.0, 0.0, 0.0,
                       0.0, 0.0, 0.0,
 angle               =  0.0, 0.0, 0.0,
                       0.0, 0.0, 0.0 /

&setvel
 mat_list = 3,
 u0 = 0,
 v0 = 0,
 w0 = 0.224580486 /

&tracers
 frame = 50*'Eulerian',
 xyz   =
 1, 0.00, 0.00, 0.025,
 2, 0.00, 0.00, 0.075,
 3, 0.00, 0.00, 0.125,
 4, 0.00, 0.00, 0.175,
 5, 0.00, 0.00, 0.225,
 6, 0.00, 0.00, 0.275,
 7, 0.00, 0.00, 0.325,
 8, 0.00, 0.00, 0.375,
 9, 0.00, 0.00, 0.425,
10, 0.00, 0.00, 0.475,
11, 0.00, 0.00, 0.525,
12, 0.00, 0.00, 0.575,
13, 0.00, 0.00, 0.625,
14, 0.00, 0.00, 0.675,
15, 0.00, 0.00, 0.725,
```

16, 0.00, 0.00, 0.775,
17, 0.00, 0.00, 0.825,
18, 0.00, 0.00, 0.875,
19, 0.00, 0.00, 0.925,
20, 0.00, 0.00, 0.975
21, 0.00, 0.00, 1.025
22, 0.00, 0.00, 1.075
23, 0.00, 0.00, 1.125
24, 0.00, 0.00, 1.175
25, 0.00, 0.00, 1.225
26, 0.00, 0.00, 1.275
27, 0.00, 0.00, 1.325
28, 0.00, 0.00, 1.375
29, 0.00, 0.00, 1.425
30, 0.00, 0.00, 1.475
31, 0.00, 0.00, 1.525
32, 0.00, 0.00, 1.575
33, 0.00, 0.00, 1.625
34, 0.00, 0.00, 1.675
35, 0.00, 0.00, 1.725
36, 0.00, 0.00, 1.775
37, 0.00, 0.00, 1.825
38, 0.00, 0.00, 1.875
39, 0.00, 0.00, 1.925
40, 0.00, 0.00, 1.975
41, 0.00, 0.00, 2.025
42, 0.00, 0.00, 2.075
43, 0.00, 0.00, 2.125
44, 0.00, 0.00, 2.175
45, 0.00, 0.00, 2.225
46, 0.00, 0.00, 2.275
47, 0.00, 0.00, 2.325
48, 0.00, 0.00, 2.375
49, 0.00, 0.00, 2.425
50, 0.00, 0.00, 2.475 /