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Title: Notes on the ExactPack Implementation of the DSD Rate Stick Solver

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## Notes on the ExactPack Implementation of the DSD Rate Stick Solver

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The DSD rate stick problem requires the solution of the level set equation

$$\phi_t + D_n|\nabla\phi| = 0$$

where $D_n$ is the detonation velocity in the shock-normal direction given by

$$D_n = D_{CJ} - \alpha\kappa$$

and $\kappa$ is the curvature of $\phi$.

The complete problem can be defined in either a planar slab configuration which sandwiches the HE between two layers of confinement materials or in an axisymmetric cylinder configuration with a cylinder of HE confined by a hollow cylinder of material. The planar slab case is calculated in $xy$-space and will use those variables in the following explanation. The axisymmetric cylinder case is calculated in $rz$-space. In the following explanation, $r$ is denoted by $x$ and $z$ is denoted by $y$ in order to consolidate the two cases into one set of functions.

### Development of the Level Set Equation

The level set function is assumed to be of the form

$$\phi = y - f(x,t)$$

and the burn front is assumed to be located at $\phi = 0$. Taking the appropriate derivatives, we obtain

$$\phi_t = -f_t$$

$$\nabla\phi = -f_x\vec{\imath} + \vec{\jmath}$$

$$|\nabla\phi| = \sqrt{1 + (f_x)^2}$$

and

$$\kappa = -\frac{f_{xx}}{(1 + (f_x)^2)^{3/2}} - n\frac{f_x}{x(1 + (f_x)^2)^{1/2}}$$

where $n = 0$ for the planar slab case and $n = 1$ for the axisymmetric cylinder case. It should be noted that the second term is undefined when $x = 0$. However, using L'Hopital's Rule, it can be shown that

$$\lim_{x\to 0}\kappa = -2f_{xx}$$

and that value is used for $x = 0$. The level set equation can then be written as

$$f_t = D_{CJ}\sqrt{1 + (f_x)^2} + \alpha\frac{f_{xx}}{1 + (f_x)^2} + \alpha n\frac{f_x}{x}.$$

### Initial and Boundary Conditions

In the planar slab case, the HE is located in the region $-R \le x \le R$, but is calculated in only the right half of this interval. In the cylindrical case, the HE is located in the region $0 \le x \le R$. The boundary conditions are the same for the two cases and consist of a symmetry boundary at the center of the HE:

$$f_x(0,t) = 0$$

and satisfaction of the DSD edge angle condition along the confinement material:

$$f_x(R,t) = -\cot(\omega_c).$$

In addition, the location of the burn front is specified at $t = 0$. Several cases are included in the solver and are described in the ExactPack documentation.

**Discretization of the Level Set Equation**

Let the subscript denote the $x$-location of a grid point:

$$x_i = i\Delta x, \qquad 0 \leq i \leq nx$$

and the superscript denote the time step. The following discretizations are used in the solver:

$$f_t(x_i^n) = \frac{f_i^{n+1} - f_i^n}{\Delta t}$$
$$f_x(x_i^n) = \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}$$
$$f_{xx}(x_i^n) = \frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\Delta x)^2}.$$

This leads to the following discretization of the level set function in the slab case:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = D_{CJ}\sqrt{1 + \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)^2} + \alpha \frac{\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\Delta x)^2}}{1 + \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)^2}.$$

In order for a discretization to be useful, it must be convergent. The usual way to show convergence is to show that a scheme is both consistent (the difference between the discretization scheme and the corresponding PDE approaches 0 as $\Delta t$ and $\Delta x$ approach 0) and stable (the solution remains bounded in some sense). In addition, the problem must be well-posed. The following sections address the consistency and stability of the proposed discretization.

**Consistency of the Discretization**

To prove consistency, we expand the function values at other nodes using a Taylor series about $x_i^n$ such as

$$f_i^{n+1} = f_i^n + \Delta t f_t + \frac{1}{2}(\Delta t)^2 f_{tt} + \cdots$$
$$f_{i+1}^n = f_i^n + \Delta x f_x + \frac{1}{2}(\Delta x)^2 f_{xx} + \frac{1}{6}(\Delta x)^3 f_{xxx} + \cdots$$

and

$$f_{i-1}^n = f_i^n - \Delta x f_x + \frac{1}{2}(\Delta x)^2 f_{xx} - \frac{1}{6}(\Delta x)^3 f_{xxx} + \cdots$$

It can then be shown that

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = f_t + \frac{1}{2}\Delta t f_{tt} + O((\Delta t)^2)$$
$$\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} = f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)$$
$$\frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\Delta x)^2} = f_{xx} + \frac{1}{12}(\Delta x)^2 f_{xxxx} + O((\Delta x)^4).$$

Substituting these into the discretization scheme gives the following equation which must be compared to the original PDE:

$$f_t + \frac{1}{2}\Delta t f_{tt} + O((\Delta t)^2)$$
$$= D_{CJ}\sqrt{1 + \left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^2} + \alpha \frac{f_{xxx} + \frac{1}{12}(\Delta x)^2 f_{xxxx} + O((\Delta x)^4)}{1 + \left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^2}.$$

Because the PDE is nonlinear, to finish the consistency argument, both this form of the discretization and the original PDE must be expanded in Taylor series, as well. We use the following expansions:

$$\sqrt{1 + x^2} = 1 + \frac{1}{2}x^2 - \frac{1}{8}x^4 + \frac{1}{16}x^6 + \cdots$$

and

$$\frac{1}{1 + x^2} = 1 - x^2 + x^4 - x^6 + \cdots$$

The PDE becomes

$$f_t = D_{CJ}\left[1 + \frac{1}{2}(f_x)^2 - \frac{1}{8}(f_x)^4 + \cdots\right] + \alpha f_{xx}[1 - (f_x)^2 + (f_x)^4 - \cdots].$$

The discretization becomes

$$f_t + \frac{1}{2}\Delta t f_{tt} + O((\Delta t)^2)$$
$$= D_{CJ}\left[1 + \frac{1}{2}\left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^2 - \frac{1}{8}\left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^4 + \cdots\right]$$
$$+ \alpha\left[f_{xxx} + \frac{1}{12}(\Delta x)^2 f_{xxxx} + O((\Delta x)^4)\right]\left[1 - \left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^2\right.$$
$$\left. + \left(f_x + \frac{1}{6}(\Delta x)^2 f_{xxx} + O((\Delta x)^4)\right)^4 - \cdots\right].$$

The difference (discretization – PDE) is

$$\Delta t\left(\frac{1}{2}f_{tt}\right) + O((\Delta t)^2)$$
$$= (\Delta x)^2\left\{D_{CJ}\left[\frac{1}{6}f_x f_{xxx} - \frac{1}{12}(f_x)^3 f_{xxx} + \cdots\right]\right.$$
$$\left. + \alpha\left[\frac{1}{12}f_{xxxx} - \frac{1}{12}f_{xxxx}(f_x)^2 - \frac{1}{3}f_x(f_{xxx})^2 + \frac{2}{3}(f_x)^3 f_{xxx} + \cdots\right]\right\} + O((\Delta x)^4).$$

Assuming that all of the derivatives are smooth across the domain, it is easy to see that the consistency condition is met by this discretization. This also shows that the discretization should be close to first-order accurate in time and second-order accurate in space.

**Stability of the Discretization**

Stability analysis is based on Fourier analysis. However, the integrals can be replaced with a simpler and equivalent procedure where we define the discretized value at a node to be the complex-valued function

$$f_m^n = g^n e^{im\vartheta}$$

where $g$ is the amplification factor, which gives the amount that the amplitude of each frequency in the solution is multiplied by in each time step. For stability, we need to show that $|g(\vartheta)| \leq 1$.

We return to the original discretization

$$\frac{f_m^{n+1} - f_m^n}{\Delta t} = D_{CJ}\sqrt{1 + \left(\frac{f_{m+1}^n - f_{m-1}^n}{2\Delta x}\right)^2} + \alpha \frac{\dfrac{f_{m+1}^n - 2f_m^n + f_{m-1}^n}{(\Delta x)^2}}{1 + \left(\dfrac{f_{m+1}^n - f_{m-1}^n}{2\Delta x}\right)^2}$$

and again apply a Taylor series expansion. Keeping only the linear terms, we obtain

$$\frac{f_m^{n+1} - f_m^n}{\Delta t} = D_{CJ} + \alpha\left(\frac{f_{m+1}^n - 2f_m^n + f_{m-1}^n}{(\Delta x)^2}\right)$$

which we use to estimate the stability of the nonlinear discretization. The constant is ignored in the analysis as it does not affect the amplification factor. Plugging in the above complex-valued function, we obtain

$$\frac{g^{n+1}e^{im\vartheta} - g^n e^{im\vartheta}}{\Delta t} = \alpha\frac{g^n e^{i(m+1)\vartheta} - 2g^n e^{im\vartheta} + g^n e^{i(m-1)\vartheta}}{(\Delta x)^2}.$$

Factoring out the common factor, this becomes

$$\frac{g-1}{\Delta t} = \alpha\frac{e^{i\vartheta} - 2 + e^{-i\vartheta}}{(\Delta x)^2}$$

or, equivalently,

$$g = 1 - 4\frac{\alpha\Delta t}{(\Delta x)^2}\sin^2\left(\frac{\vartheta}{2}\right)$$

which must satisfy the condition $|g(\vartheta)| \leq 1$. Thus,

$$-1 \leq 1 - 4\frac{\alpha\Delta t}{(\Delta x)^2}\sin^2\left(\frac{\vartheta}{2}\right) \leq 1$$

and

$$0 \leq \frac{\alpha\Delta t}{(\Delta x)^2}\sin^2\left(\frac{\vartheta}{2}\right) \leq \frac{1}{2}.$$

Since $\sin^2\left(\frac{\vartheta}{2}\right) \leq 1$, the stability condition becomes

$$\frac{\alpha\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$$

or

$$\Delta t \leq \frac{(\Delta x)^2}{2\alpha}$$

Typically, the time step is chosen to be some fraction of this condition, especially in the case of a nonlinear equation. I have chosen to use 80% of this time step, even though the calculations appeared to be stable at the full time step. The stability condition is often called the CFL (Courant-Friedrichs-Lewy) condition.

**Boundary Conditions**

Because the DSD solution is almost entirely dependent on the boundary conditions, it is necessary to use a mathematically defensible treatment of them. The symmetry boundary condition

$$f_x(0,t) = 0$$

is discretized using a ghost node, which is set to the value

$$f_{-1}^{n+1} = f_1^{n+1}.$$

This boundary condition is second-order accurate in space. It also makes physical sense, as the node at $x = 0$ should be allowed to stay slightly ahead of these two nodes, as would be seen in a propagating wave.

There are many choices of discretizations to implement the boundary condition at the confinement boundary:

$$f_x(R,t) = -\cot(\omega_c).$$

Previous versions of codes to solve this problem used a ghost node and a discretization to match the overall scheme given above:

$$f_{N+1}^{n+1} = f_{N-1}^{n+1} - 2\Delta x \cot(\omega_c)$$

where $R = N\Delta x$. While this is mathematically consistent with the first derivative, it causes problems with the second derivative and curvature because it does not move the boundary node to where it truly belongs. As a result, very large curvatures are calculated at this boundary and the discretization scheme is no longer stable. In the previous codes, both maximum and minimum limits were placed on the curvature to control its effect on the calculation. Since the curvature at the boundary is the very thing that is supposed to drive the solution, it is hard to justify using these limits from a mathematical perspective.

It makes mathematical and physical sense to use a one-sided scheme that places the boundary node where it needs to be to satisfy the boundary condition:

$$f_N^{n+1} = f_{N-1}^{n+1} - \Delta x \cot(\omega_c).$$

While this choice is only first-order in space, it does not affect the stability of the scheme and the boundary curvature can now directly drive the solution on the adjacent nodes.

**Conclusion**

It has been shown above that the discretization scheme implemented in the ExactPack solver for the DSD Rate Stick equation is consistent with the Rate Stick PDE. In addition, a stability analysis has provided a CFL condition for a stable time step. Together, consistency and stability imply convergence of the scheme, which is expected to be close to first-order in time and second-order in space. It is understood that the nonlinearity of the underlying PDE will affect this rate somewhat.

In the solver I implemented in ExactPack, I used the one-sided boundary condition described above at the outer boundary. In addition, I used 80% of the time step calculated in the stability analysis above. By making these two changes, I was able to implement a solver that calculates the solution without any arbitrary limits placed on the values of the curvature at the boundary. Thus, the calculation is driven directly by the conditions at the boundary as formulated in the DSD theory. The chosen scheme is completely coherent and defensible from a mathematical standpoint.