On one approach to solving a multiscale problem with a kink

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Abstract

This contribution aims to demonstrate a method of application of COMSOL to solve a multiscale problem whose essential feature is a kink with an unknown configuration. The search for its shape and details of its structure is the main task of the study.

This paper demonstrates the approach within the example of a stationary partial differential equation with strong nonlinearity. Its solution that we look for is close to zero far from the origin of coordinates and close to a constant value within some region not far from the origin. A kink of a complex, unknown configuration separates these two domains. The lateral size of the area with the nonzero solution is about a few hundred times larger than the kink width. The latter determines the multiscale nature of this problem.

An approach is proposed using the (i) relaxation method. It consists in passing from the static equation - to the dynamic one. The relaxation method makes use of the fact that the solution of the dynamic equation converges to a fixed point. The latter represents the solution of the static equation. Thus for a large enough solution time, *t*, one can expect to be close to the solution of the static equation.

The relaxation method itself is, however, not enough. To resolve the kink region, one should supply it with (ii) the Adaptive Mesh Refinement feature switched on. The Adaptive Mesh Refinement can be tuned to build several meshes during the Study such that in the kink region, each next mesh is denser than the previous one while leaving the mesh coarse away from the kink.

One needs to supplement this by (iii) generating multiple Studies, each next of them taking the result of the previous one as the initial condition, each of them possessing the Adaptive Mesh Refinement feature.

This strategy brings one to a successful solution of the problem.

Introduction

In many brittle materials, high stress forming at the crack tip during the solid loading gives rise to a phase transformation. The latter takes place at the vicinity of the crack tip. Figure 1 shows an example of such a local phase transformation at the crack tip in a martensitic-austenitic alloy.
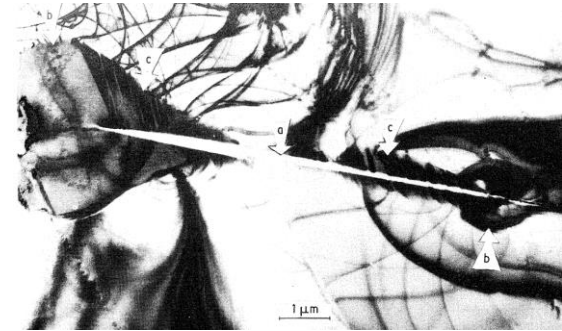

Figure 1. Local phase transitions (b, c) at both tips of the crack (a)

An order parameter, *u=u(x,y)*, can describe the phase transformation. The latter is equal to zero in the initial phase and is unequal to zero in the transformed phase. The order parameter obeys an equation

$$F(u, a, v) = \Delta u + v \frac{\partial u}{\partial x} - [a - U(x,y)]u +$$

$$+u^3 - u^5 = 0 \qquad (1)$$

where the function

$$U(x,y) = \frac{\sqrt{\sqrt{x^2+y^2}+x}}{\sqrt{x^2+y^2}} \qquad (2)$$

describes the influence of the crack tip stress on the order parameter. In equation (1), *a* and *v* are parameters. All the coordinates, parameters, and dependent variable are dimensionless.

This equation can be solved numerically. One of such solutions we show in Fig. 2. The distribution, *u(x,y)*, is very close to a kink. It exhibits a very gently sloping roof and a boundary where the order parameter dramatically drops to zero from the roof value. One can see that the dimension of the transformed area is between a few hundred dimensionless units, while the width of the kink is about a few such units — one faces, thus, with a multiscale problem.

On the other hand, since the shape of the solution is clear, the main question the solution should answer is what is the configuration of the kink.

This paper describes the approach enabling one to find solutions possessing kinks of nonlinear equations like Eq. (1).

The Relaxation Method

The solution describing the process zone shows up in the vicinity of the crack tip. Natural boundary condition describing such a local solution is $u(\infty) = 0$. To solve this problem numerically, one separates
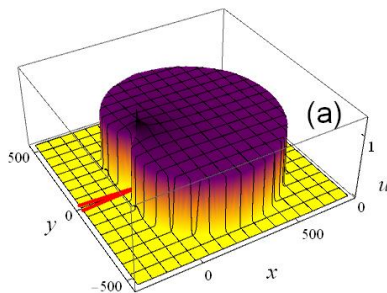

Figure 2. The order parameter, $u(x,y)$ obtained by the COMSOL simulation. The red lines schematically show the position of the crack tip.

domain, Ω, which is considerably larger than the size of the zone within the kink, such that at its boundary, $\partial\Omega$, the order parameter is very small. Let us impose the Dirichlet condition at $\partial\Omega$: $u(x,y)|_{\partial\Omega} = 0$.

One can, further, see that the equation of state (1) is highly nonlinear. Also, *u=0* gives the solution to this equation $F(0,a) = 0$. One is tempted to solve equation (1) in the domain Ω with the boundary condition $u(x,y)|_{\partial\Omega} = 0$. In this case, however, COMSOL always returns the trivial solution, *u(x,y)=0*. The latter takes place because the trivial solution is one of the solutions to equation (1).

The workaround is to start from some arbitrary initial distribution, $u(x,y) \neq 0$, and to make iterations successively converging to the desired nontrivial solution of (1).

One can most easily do such a procedure by the so-called, relaxation method. Instead of the equation (1), one takes the time-dependent equation

$$\frac{\partial u(x,y,t)}{\partial t} - F[u(x,y,t),a] = 0 \qquad (3)$$

Here *t* is an auxiliary parameter, a pseudo-time. The method is based on the observation that the solution, *u(x,y,t)*, of Eq. (3) converges to the

solution, *u(x,y)*, of the stationary equation with $t \to \infty$ as $u(x,y,\infty) = u(x,y)$. For this reason, instead of the stationary problem, here we will solve a time-dependent equation for $u = u(x,y,t)$

$$\frac{\partial u}{\partial t} = \Delta u - [a - U(x,y)]u + u^3 - u^5 \qquad (4)$$

with the initial condition $u(x,y,0) = u_0(x,y) \neq 0$, and zero Dirichlet boundary conditions described above. We, further, look for a solution at a high value of time, *t*.

More details on the relaxation method in application to nonlinear PDEs one finds in the paper [1].

Solution Method

Step 1

Let us start the Comsol 2D model and the Time-dependent solution template. Let us define the parameters *a=0.23*, *v=0.2*, *T=1000* and *deltaT=100*. The two latter parameters define the time stepping.

Let us further introduce a smooth rectangle, *rect1* provided by the COMSOL standard analytical functions. It should have a lower limit at 0 and the upper one at 200. One will use it as the initial condition.

The domain represents a rectangle whose size exceeds the dimension of the expected solution. One determines the proper size by trial and error. The equation has the mirror symmetry $y \to -y$ enabling one to only study the problem at *y>0*. Zero Dirichlet boundary conditions are fixed on its three boundaries, while at *y=0* (the mirror plane) one requires the no-flux condition. The equation is comfortable to define in a general form with the standard Γ, e_a=0, d_a =1, and the free term *f*:

$$f = v * ux - \left(a - \frac{sqrt(sqrt(x^2 + y^2) + x)}{sqrt(x^2 + y^2 + b)}\right)u + u^\wedge 3 - u^\wedge 5$$

Where *b=0.0001* is a regularization constant. Finally, one defines the initial distribution using the smooth rectangle introduced earlier, by fixing "Initial value for u "→*rect1(x^2+y^2)* in the "Model 1/General Form/ Initial values > Settings/Initial values."

The next step is to make the initial mesh. The latter should be coarse enough. Then we will gradually refine it such that it only becomes finer in the places where the gradient of the solution is steep, while otherwise, it stays coarse. Let us choose Physics-controlled/Normal mesh (Fig. 3).

The next step is the Study. The time-stepping we define as the range(0,deltaT,T) meaning that the simulation runs from *0* till *T* and each *deltaT* the solution is stored.
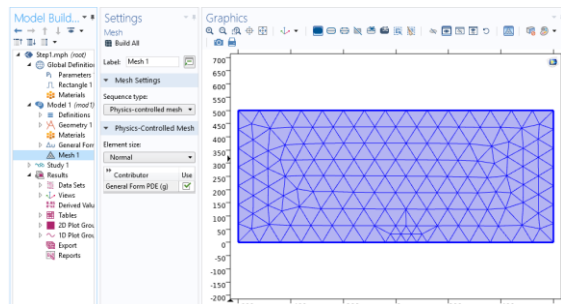

Figure 3. The initial Physics-Controlled/Normal mesh.

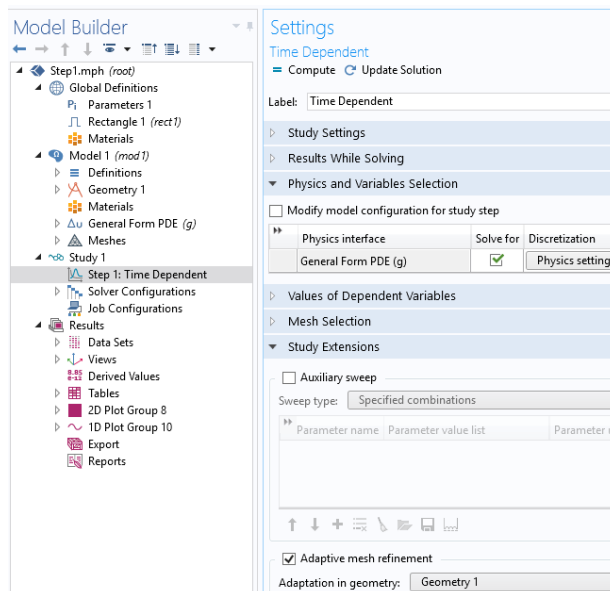It is essential to check the Adaptive Mesh Refinement (AMR) under Study Extensions (Fig. 4).

Figure 4. One should check the Adaptive mesh refinement checkbox

After one has done this, one can fine-tune the AMR. To do this, let us right-click "Model Builder/Study" and select "Show Default Solver" from the drop-down menu. This operation makes a node "Adaptive Mesh Refinement" visible under "Study/Solver Configurations/ Solution/ Time-Dependent Solver." Let us click the AMR node and vary its parameters in the Settings page. The best values of these parameters are problem-specific. One can play with them and choose the combination optimal for the equation in question. For the problem considered here, the optimal AMR parameters found by trial and error one finds in Fig. 5. Please pay attention that the error indicator is the absolute value of the solution gradient.

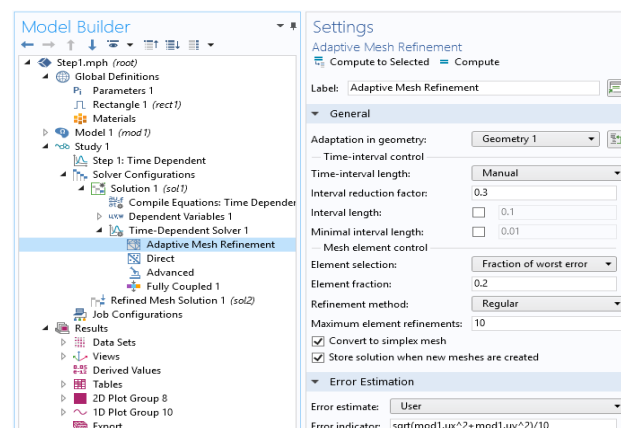Decreasing it ten-fold makes the AMR more sensitive.

Figure 5. Fine-tuning of the Adaptive Mesh Refinement

Now, let us solve the problem and look at the meshes formed after the solution. In Figure 6, we displayed refined Mesh 11. This refinement is, however, still much too rough. Therefore, one needs to repeat the procedure.
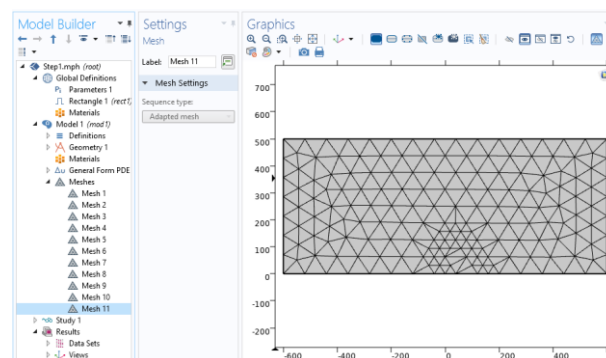

Figure 6. The refined Mesh 11 after Study 1

Step 2

Let us make a new study. Go to the "Ribbon/Add Study" and choose "Time-Dependent." Now it is important that in this second study, the time-stepping parameters are as follows: *range(T,deltaT,2*T)*. It is further important that COMSOL gets the instruction to take the previous solution as the initial value and start with the solution corresponding to the very last moment of the previous study.

Further, one should select the very last mesh (in this case, Mesh 11) as the starting one. Figure 7 shows these settings. As in the previous case, one checks the checkbox "Study Extensions/Adaptive mesh refinement" visualizes the node "Adaptive mesh refinement" and fine-tunes its parameters. We already described this fine-tuning in Step 1, and one should tune them analogously. All these settings are important features of the approach.

Let us now compute. The 2D plot of the result we displayed in Fig. 8.

Let us now check the convergence in "Results/ DerivedValues/SurfaceIntegration," where we choose the whole Domain 1 and "Study 2/Refined mesh solution" as the Data set to see the result for the second study. Let us integrate the gradient of the solution squared over the domain Ω:

$$ J = \int (\nabla u)^2 \, d\Omega $$

It is a very sensitive convergence indicator for the problems with the kink. We can evaluate it for all times saved during the study and plot the resulting table (Fig. 9). One can see that the solution still exhibits considerable growth. The latter indicates that it is still far from the fixed point, *u(x,y)*. The same conclusion one can make looking at the boundary configuration of the solution. Indeed, it exhibits sharp corners and straight portions of the boundary, while in the correct solution one expects a smooth, continuous boundary. Such observations mean that one should repeat the procedure more times.
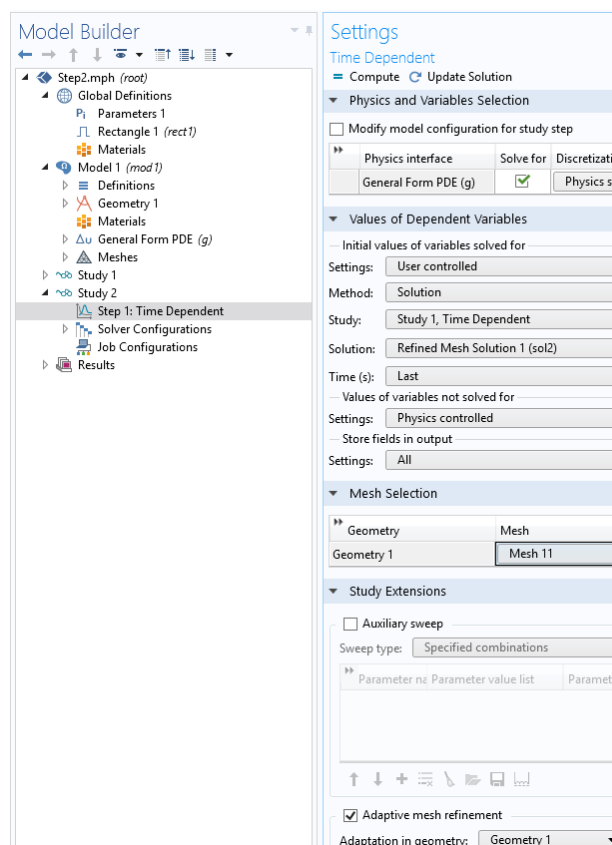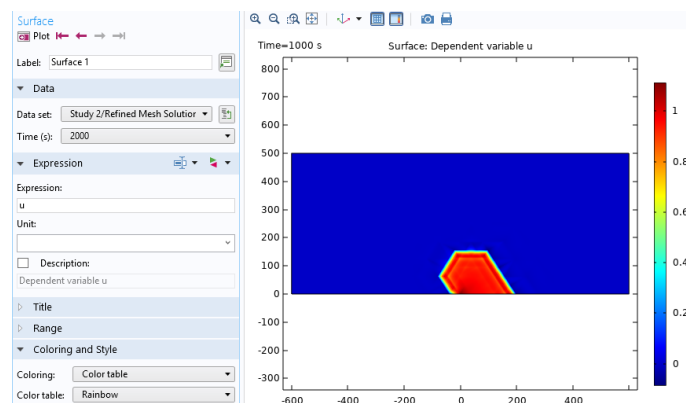

Figure 7. The settings for Study 2

Figure 8. 2D Plot Group/Surface for Study 2/Refined Mesh Solution

The last step

The number of studies required for the ultimate convergence is problem-specific. Moreover, it also depends on the values of parameters (in the present case – on *a* and *v*). One finds this dependence especially manifested if the nonlinear equation in question exhibits a bifurcation. It is this case that takes place with Eq. (1). As soon as the parameter *a* is close to its bifurcation value, one needed up to a few hundreds of Studies to achieve the convergence. In contrast, far from this value, five to ten studies were enough.

Now, let us have a look at the final stage of the solution. In the present case (*a=0.23* and *v=0.2*), the
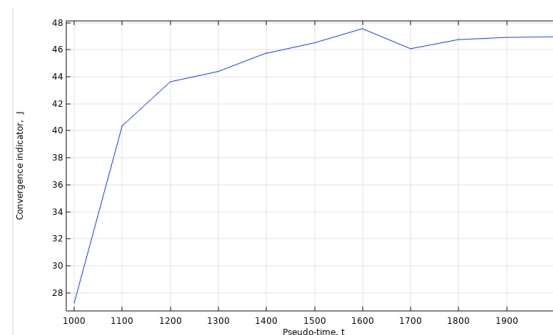

Figure 9. The convergence indicator of the solution, *J*, versus the pseudo-time, *t*.

solution has been repeated 23 times until the boundary became smooth, the distribution, *u(x,y)*, stopped to vary in its size, and the indicator exhibited a convergence. The coincidence of the numbers *a=0.*23 with the 23 Studies is occasional. One can see the 2D plot of the solution of Study 23 in Fig. 10.
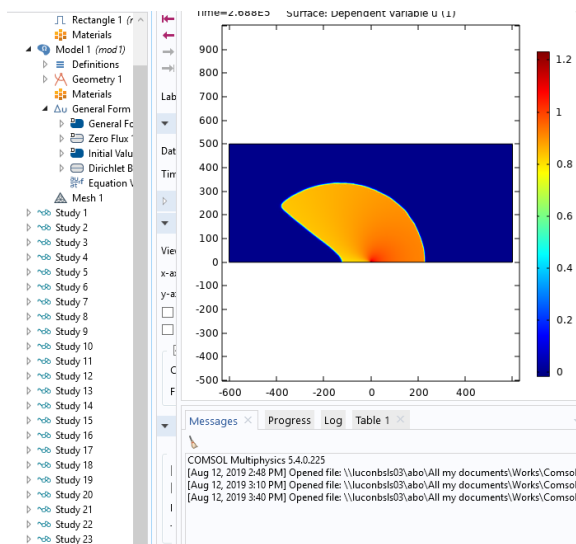
Figure 10. 2D Plot Group/Surface for Study 23

The solution exhibits a smooth boundary, which is one of the indicators showing that it is close to the correct one.

In the course of the solution, Comsol has built 211 meshes. The view of the last mesh one finds in Fig. 11. One can see that it is very dense at the kink and sparse otherwise.

Simultaneously, the integral of the square of the gradient, $ux^2 + uy^2$ over the domain finally reaches the horizontal asymptotics (Fig. 12). All these properties indicate that the solution of the dynamic equation is already close to the desired solution of the static one.
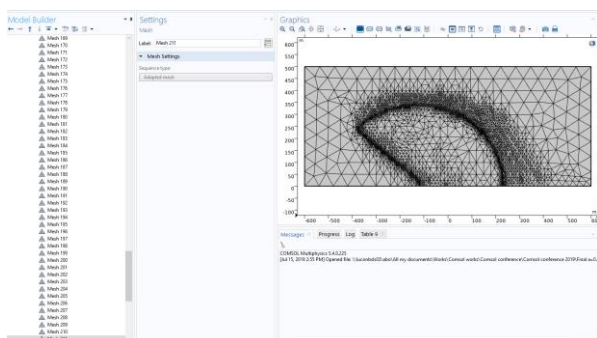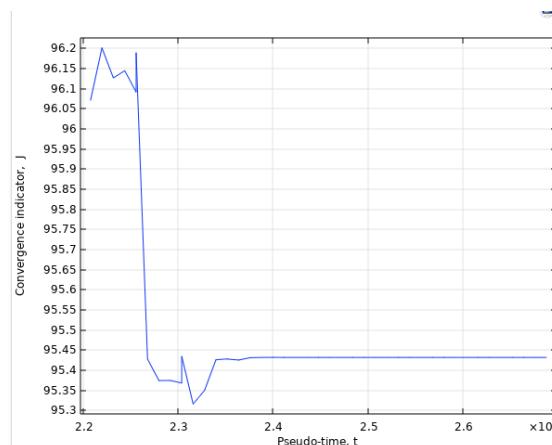

Figure 11. The form of the last mesh Nr. 211

Figure 12. The convergence indicator reaches horizontal asymptotics during the Study 23

Summary

To summarize, COMSOL enables one to combine the relaxation method with the Adaptive Mesh Refinement. Applying multiple studies, one achieves a good convergence of the solution of a highly nonlinear problem exhibiting a steep kink. The penalty is the large time required for multiple simulations.

References

1. A. Boulbitch, Pseudo-Dynamic Approach to the Numerical Solution of Nonlinear Stationary Partial Differential Equations. *The Mathematica Journal*, **20**, 1-21 (2018)