Computational Continuum Mechanics
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Lecture – 35
Line Search Method

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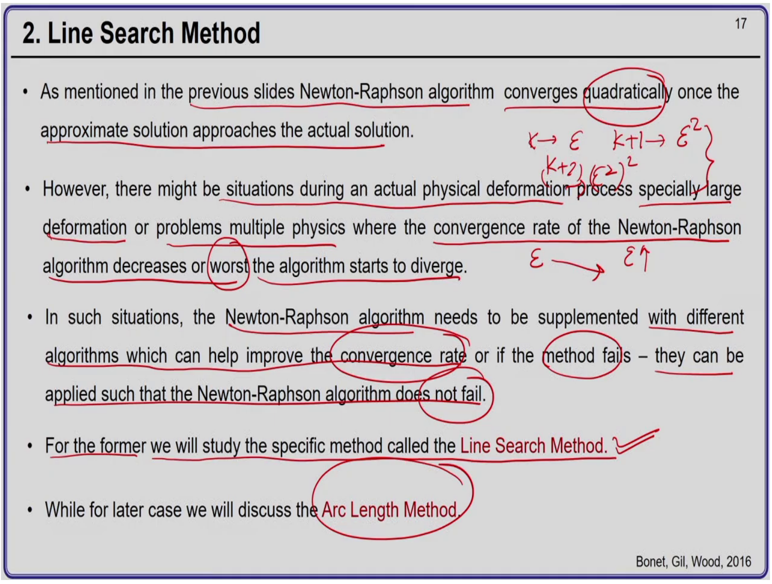

So, when Newton – Raphson method faces some convergence issues so, we will employ a technique called line search method to prevent the divergence of the algorithm.

Now, to recapitulate we have mentioned in the previous slides that the Newton – Raphson algorithm converges quadratically; once the approximate solution approaches the actual solution. So, quadratically means the error if say in the step K is epsilon then in K plus 1th step the error would go down by epsilon square and then for example, in K plus 2 it will go down by epsilon square ok. So, this is only when you are near to the actual solution.

However, there might be situations during an actual physical deformation process especially when dealing with large deformation problems or problems with multiple physics where you will find that the convergence rate of the Newton – Raphson method decreases or worse the algorithm will start to diverge ok. So, not only you will find that the convergence rate has gone down that the error epsilon does not go down fast enough ok, but rather you will can also find in the worst case that your error starts to increase ok. So, which means that the Newton – Raphson algorithm has start to diverge.

In that case you have to supplement the Newton – Raphson algorithm with different algorithms to improve the convergence rate or if the method fails you have to apply algorithms which can prevent the failure of the Newton – Raphson algorithm ok.

Now, for the former that is when the convergence rate of the Newton – Raphson algorithm is slow, then we will study one specific method which is applied which is called the line search method ok. And, for the later case where the method starts to fail then we will apply what is called the arc length method ok.

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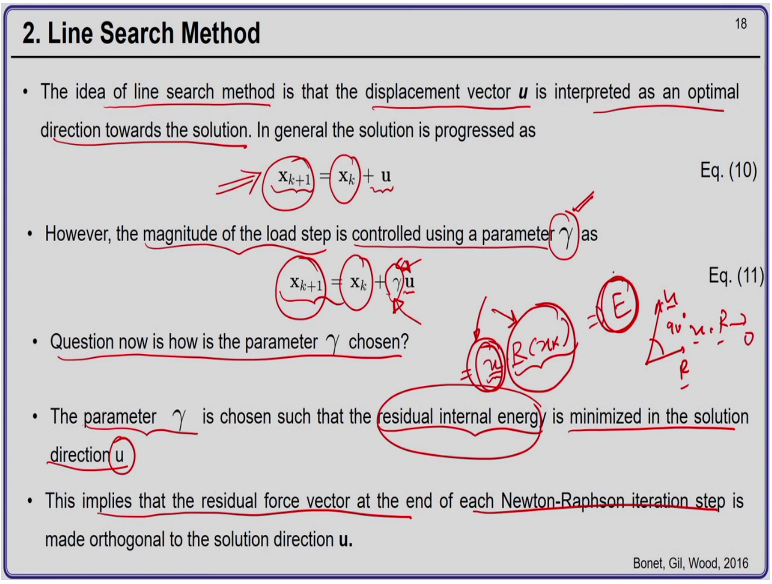

So, let us see the line search method ok. So, the idea of line search method is that it views the displacement vector u as an optimal direction towards the solution ok. So, we know that the solution at k plus 1 is updated using the solution at k plus the increment u ok.

Now, what happens in line search method is that the magnitude of the load step is controlled by a parameter that is a scalar parameter gamma as given here ok. So, the solution at Newton – Raphson steps k plus 1 is equal to the solution at step k plus gamma times solution u ok. Now, our objective is to find out this gamma ok.

Now, the question is how do we actually find out this gamma ok. To do this we follow the idea that gamma would be a value that will make the residual energy minimum in the solution direction u ok. So, this u will be this gamma will be such that the residual internal energy that is the residual strain energy which is given by the displacement vector u dotted with the residual force vector r is minimized ok.

So, this will imply that the residual force ok; so, if this is the energy so, minimizing this energy for a given value of u given vector u would mean that the residual force vector R at the end of each Newton – Raphson iteration step is made orthogonal to the solution diagonal then only because this is a vector and, this is a vector and if this has to be minimized therefore, u and R these both have to be orthogonal to each other then only this u dot R will approach 0 that is the residual energy will be minimized ok.

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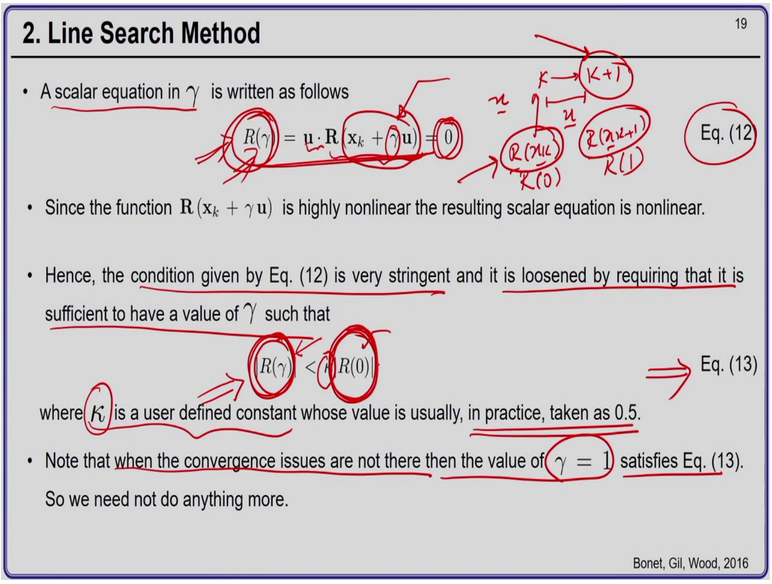

So, how do we do that? Ok. So, we write a scalar equation in gamma ok. So, this R gamma is a scalar equation which is obtained by taking the displacement vector u dotted with the residual vector R evaluated at x k plus 1 plus gamma u. Remember, we already know u because we have solved the Newton – Raphson iteration from K to K plus 1. So, at K plus 1 we know this increment in the displacement and we know the residual with force vectors at K and K plus 1.

And, now, what we have done we have found out that our Newton – Raphson algorithm is diverging at K plus 1 or if the convergence is very slow there has to be a certain criteria based on which you can say that the Newton – Raphson algorithm is converging very slowly or it is diverging. In that case we take u dot R evaluated at x k plus gamma u. So, in this equation the only unknown is this unknown scalar gamma ok.

Now, this residual force vector is a highly non-linear function ok. Therefore, this equation R gamma is a highly non-linear equation that we need to solve ok. Therefore, to make this R gamma equal to 0 is a very stringent condition ok. So, this condition given by equation number 12 is a very stringent condition and we can loosen this condition by requiring that instead of making R gamma go to 0, we will be happy if the absolute value of R gamma is less than some scalar kappa times the absolute value of the function R gamma at gamma equal to 0 ok.

So, R 0 is basically so, this is R 0 and this is R 1 ok. If you put gamma equal to 0 you get residual at x K and if you put gamma equal to 1 you get residual at R x K plus 1 ok. So, we require that we choose a value of gamma such that the absolute value of this function R gamma is less than kappa times the absolute value of the function R gamma evaluated at gamma equal to 0 ok.

And, now this kappa is basically your user defined constant ok. So, at the start of the simulation the user can define what is this value of kappa and usually in practice it is taken as 0.5. So, what it means is I will be happy with that value of gamma which makes the residual internal energy less than 0.5 times of the residual internal energy at R 0 ok.

Now, note that when the convergence issues are not faced ok, so, if you the Newton – Raphson algorithm is converging nicely from K to K plus 1 then the value of gamma equal to 1 satisfies equation number 13 and we need not do anything more. But, if the Newton –

Raphson method is diverging or the Newton – Raphson method is converging very slowly according to certain criteria then we have to find out the value of gamma.

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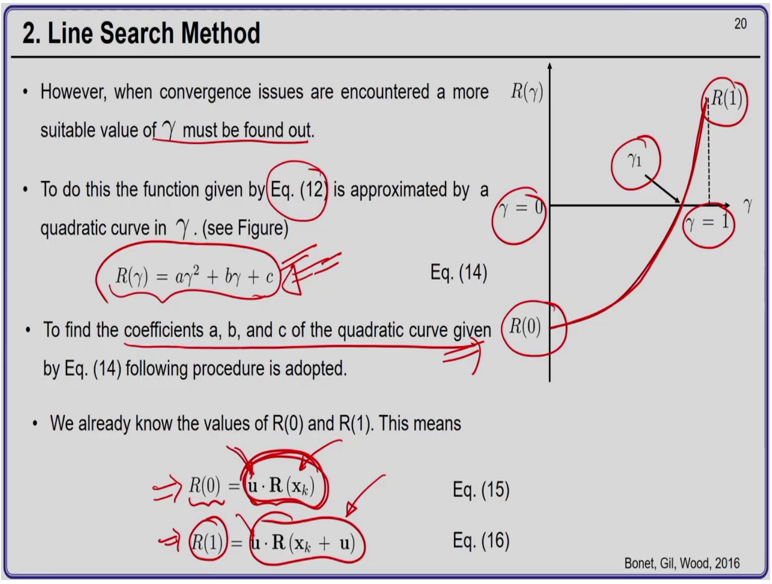

So, gamma must be found out and how do we do that? We do that by approximating the function given by equation 12 if you see this is equation 12 ok. So, equation 12 is a unknown function in gamma ok. Remember R is a highly non-linear vector and therefore, R gamma will be highly non-linear function in gamma which is not known or we cannot actually derive that.

So, what we do is we approximate R gamma as a quadratic function ok. A quadratic function given by a gamma square b gamma plus c where; a, b, c are the constants that we need to determine ok. So, you can see this figure ok. So, R 0 is the value of the function at gamma equal to 0 and R 1 is the value of function at gamma equal to 1 ok. And, now this increasing in this value of R denotes there is a divergence there is some convergence issue.

So, we like to find out that value of gamma equal to gamma 1 where our condition given by equation 13 will be satisfied. So, what will be that value of gamma let us find out ok. In order to find out that value of gamma first we need to determine the value of the coefficients a, b and c. Once we have determine the value of the coefficient a, b, c finding that value of gamma would correspond to finding the root of this equation ok.

Remember, if you see equation number 12 ok. So, getting R gamma equal to 0, means that gamma should be the root of this function R gamma ok. So, to find out a, b, c what we know is that at gamma equal to 0 R 0 is u dot the residual force vector at x k. Now, this 2 vectors we know from our Newton – Raphson iteration ok. We have already calculated this residual and we already have found out this displacement vector and at gamma equal to 1 R 1 is u dot R x k plus u and we already have found out x k plus u and this u ok.

Now, we know R 0 and R 1, there are two conditions which are known, but because this is a quadratic equation there are three unknowns a, b, c we need one more condition.

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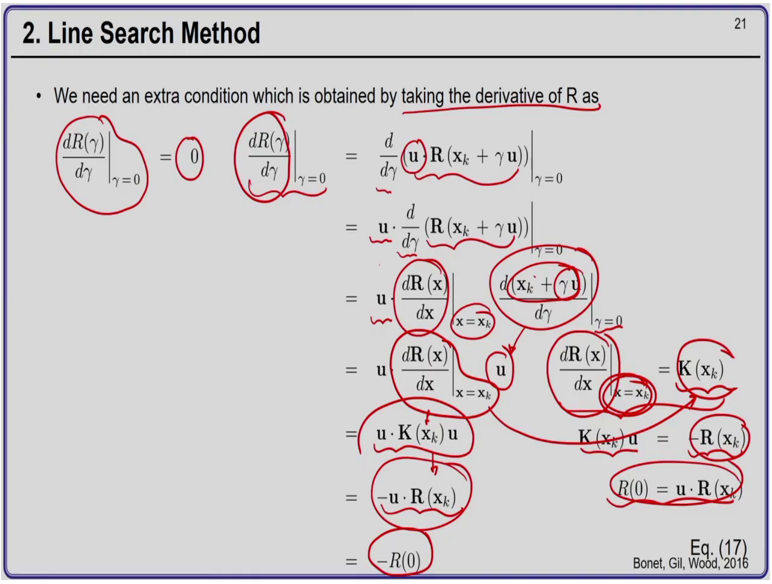

And, that one more condition is obtained by taking the derivative of function R with respect to gamma and then setting gamma equal to 0. Now, let us take the derivative of R with respect to gamma ok. Taking derivative with respect to gamma we have d by d gamma of u dot R x k plus gamma u ok. So, because u does not depend on gamma I can take it outside and then I have u dot d by d gamma of R x k plus gamma u ok.

Now, I can use the chain rule and using chain rule I get u dot dR by dx evaluated at x k into d by d gamma of x k plus gamma u evaluated at gamma equal to 0 ok. And, then what I get is this term only the second term has gamma so, it reduces to u ok. And, now from our derivations we know that the derivative of the residual force vector with respect to the current position and evaluated at the current position x k is nothing, but the tangent matrix evaluated at x k.

So, this dR by dx evaluated at current position is nothing, but K into u and that is what we substitute here. So, we get u dot K x k u, but also we know that K into u is nothing, but minus of the residual at current position ok. So, K into u is nothing, but minus of u dot R x k and this we know from our previous equation number 15 that u dot R evaluated at current position is nothing, but R 0 ok.

So, u dot R x k equal to R 0 therefore, the derivative of R with respect to gamma evaluated at gamma equal to 0 is nothing, but equal to minus R 0 ok. Now, I have three conditions and now, I am in position to find out the three coefficients of the quadratic equation a gamma square plus b gamma plus c ok.

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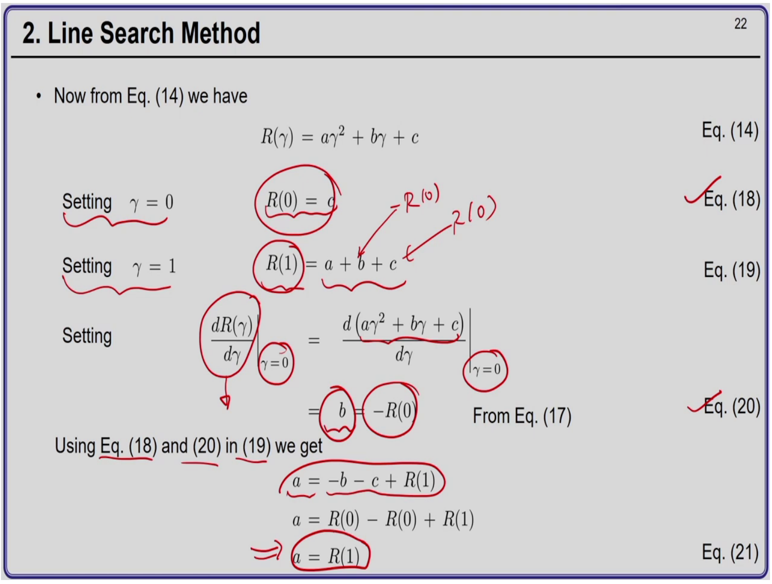

So, now from equation 14 we have this quadratic equation that approximation of R gamma is a gamma square plus b gamma plus c and now, if I set gamma equal to 0 I get R 0 equal to c because these two terms will go away and R 0 will become equal to c. So, one of the coefficient c is nothing, but R 0 that is the residual internal energy at gamma equal to 0.

Now, if I set gamma equal to 1 I get R 1 as sum of a plus b plus c ok. Now, if I take dR by d gamma and set gamma equal to 0 I get d by d gamma of a gamma square plus b gamma plus c is evaluated at gamma equal to 0 and this gives me b. And, from my previous discussion on the previous slides I know that dR by d gamma evaluated at gamma equal to 0 is nothing, but minus R 0 ok. So, I get my second coefficient b as minus R 0.

Now, you see from equation 18 and equation 20, if I substitute b at minus R 0, c as R 0 I will get a which is nothing, but equal to R 1 ok. So, a will be equal to minus b minus c plus R 1; if I substitute 18 and 20 in equation number 19 and if I simplify I will get a as R 1 ok.

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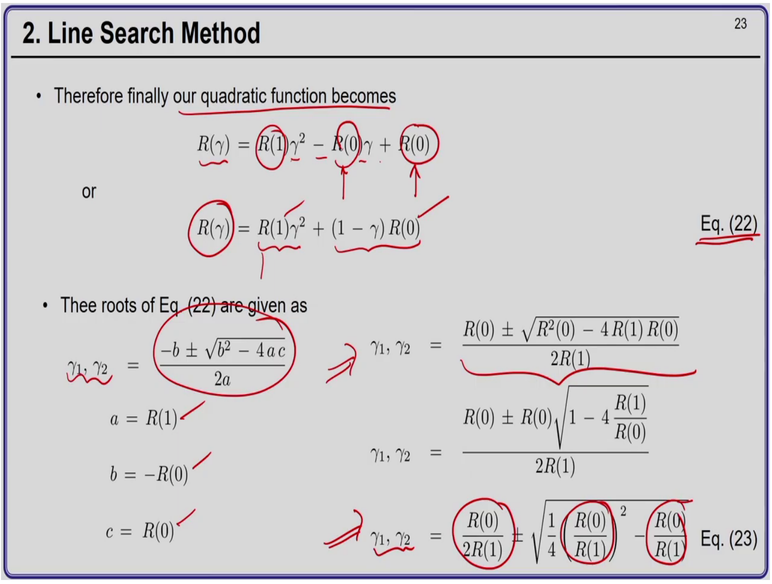

Therefore, our quadratic function now becomes R of gamma R 1 into gamma square minus R 0 into gamma plus R 0 ok, which I simplify then my quadratic function becomes R 1 into gamma square plus 1 minus gamma into R 0, ok. Now, I can find out the so, I know R 0, R 1, so now I can find out the root of the quadratic equation given by 22 ok.

So, the roots of this equation gamma 1 and gamma 2 because it is a quadratic equation it will have two roots will be equal to minus b plus minus root over b square minus 4 ac divided by 2a ok. So, a is R 1, b is minus R 0 and c is R 0. If I substitute so, a is R 1; b is minus R 0; c is R 0 and if I substitute a, b, c in this particular equation I will get my gamma 1 and gamma 2 as following ok.

Now, if I do a little more manipulation I will get gamma 1 and gamma 2 as R 0 by 2 R 1 plus minus root over 1 by 4 R 0 by R 1 the whole square minus R 0 by R 1 ok.

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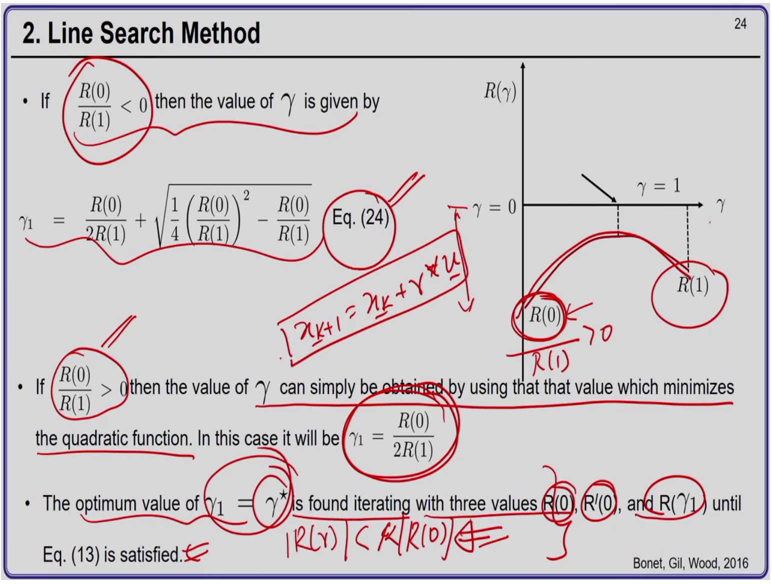

Now, there can be two cases. In the first case R 0 by R 1 may be less than 0 in that case if you have less than 0, then your gamma 1 will be equal to that given by equation number 24 ok. However, if your R 0 by R 1 is greater than 0, that the residual strain energy at R 0 divided by the residual strain energy at R 1 that is gamma 0 and gamma 1 if the ratio is more than 0 which means R 1 is less than R 0 then you will have a curve something like this.

In that case, you will not have any root and then gamma can simply be obtained by taking the value which minimizes the quadratic function and this gamma is taken as R 0 by 2R 1 ok. So, if you have R 0 by R 1 which is less than 0, then your gamma will be given by equation 24 and if you have R 0 by R 1 greater than 0 then your gamma 1 will be R 0 by 2R 1 ok.

And, then the optimal value of gamma that is gamma star will be found out by iterating the three values R 0, R dash 0 and R gamma one until equation number 13 that is R gamma less than kappa times R 0 is satisfied ok. So, this you have to carry out iteratively till you have found out the particular value of gamma that is gamma star for which your equation number 13 is satisfied.

If you have found out that value where this equation is satisfied you take that value of gamma calculate your residual and your solution x k plus 1 then will be x k plus gamma star u ok. That is how and then you can proceed to the next Newton – Raphson iteration step ok.

Thank you.