On the use of time step prediction

CODE_BRIGHT TEAM

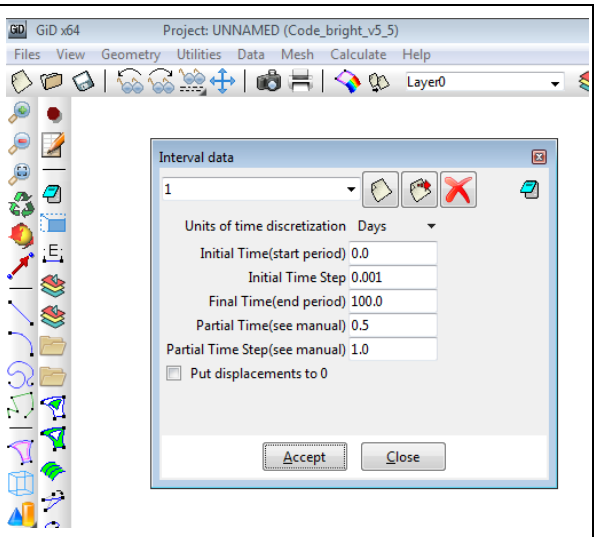
Sebastià Olivella

Contents

1 Introduction

CODE_BRIGHT uses dynamic time step variation under certain control conditions. In general, time step will tend to increase because time step is continuously increased by a factor of 1.4.

Manually, time step is given in a general card (Interval data window) with 5 values for each time interval:

Time begins at 0 days (Initial time or TIMEI) and calculation will start with and initial time step of 0.001 (Initial Time Step or DTIME). Calculation should continue until 100 days (Final Time or TIMEF). Time step will increase until 0.5 (Partial time or TIME1) from the initial value of 0.001 (DTIME). After 0.5 days (TIME1), time step can increase until it reaches the value of 1.0 (Partial Time Step or DTIMEC), which is the maximum time step. TIME1 can be equal to TIMEI or to TIMEF.	

Initial Time for second interval should be set equal to Final Time of the first interval. And so on.

Convergence failure or large variations of unknowns

When the maximum number of iterations (user defined value) is reached without convergence being achieved, current time step is rejected. A new time step is calculated by reducing the current one and new calculations are carried out. In this case time step is reduced by a factor of 2 as there is no additional information to use other values.

When a variable shows systematic values of corrections that increase during Newton Raphson iterations, the current time step is rejected and a smaller one is considered. Again a reduction by a factor of 2 is considered.

When a variable undergoes a large correction during Newton Raphson calculations, the calculations for a given time step are stopped. Time step is reduced using a scaled value which is obtained from the large variation obtained and the user defined maximum variation permitted. For instance if temperature variation is permitted up to 1^{o} C and corrections indicate a variation of 3^{o} C, time step would be reduced by a factor or 3. A lower bound is considered.

Other aspects

A projection is used to set the initial value of variables for the forthcoming time step. A very small time step will tend to reduce the number of Newton Raphson iterations until a value of 1.

In principle, a time step prediction method or algorithm can be made sufficiently strict so that the number of NR-iterations is one for all time steps. Although this solution seems attractive (because the errors are small and the possibility of failure practically disappears), the CPU time required is very large. Although a very small time step

calculations is not competitive, it can be used as a reference solution for comparison in a study of errors. This reference solution can be obtained using a time step prediction scheme based on a very low error, or it could be obtained manually. The latter is not easy because calculations normally have different periods with different requirements (for instance, heating and cooling periods require very small time step).

The Newton Raphson algorithm shows quadratic convergence. This means that corrections (and errors) decrease in a quadratic way for each new NR-iteration carried out.

A case with 1 NR-iteration corresponds to the maximum CPU time required for a given mesh and equations because it uses the minimum time step. In general, using 2 NR-iterations per time step will reduce the CPU time by a factor of 4 and using 3 NR-iterations per time step will reduce CPU time by a factor of 9 (assuming a direct solver is used).

Model to use as test case

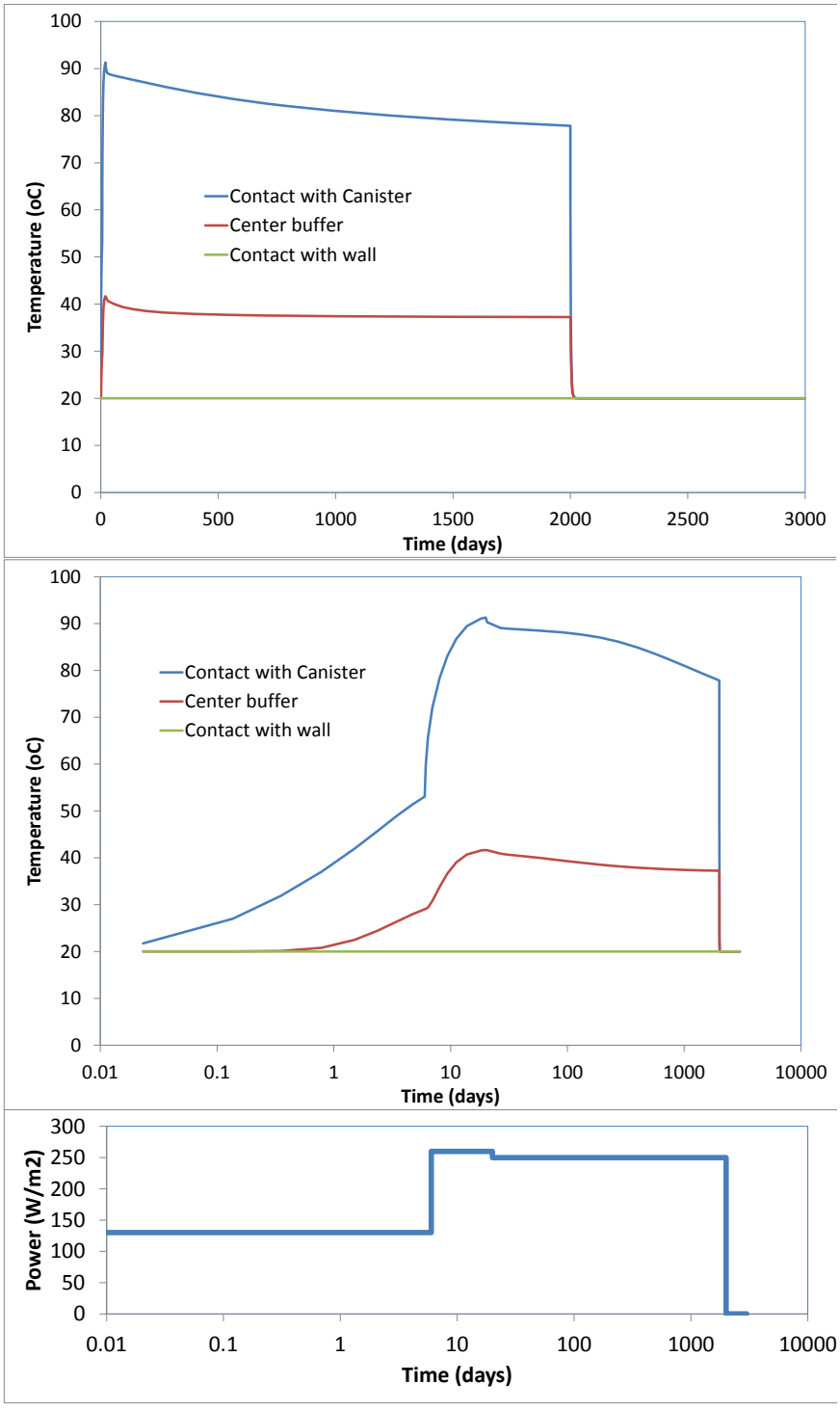
A simulation of a typical Mock-Up experiment (a simulated waste surrounded by unsaturated clay) is used to do several run tests to determine various aspects such as the error of results, the CPU time and the number of iterations.

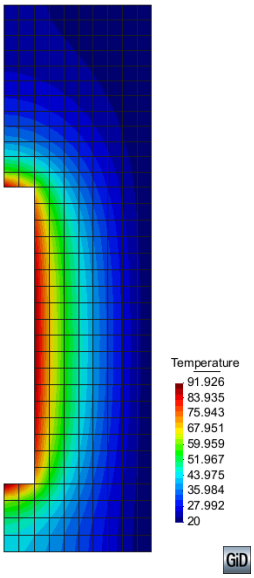
The geometry of the model is very simple. Boundary conditions are simple as well. Normal displacements are prescribed on all boundaries. Heating takes place on the inner boundary (representing the heating effect of a canister) and water pressure is prescribed on the outer boundary (representing the hydration effect from the rock).

Time days	*Time seconds*	*Boundary condition changes*
0 to 6	0 to 5.184×10^{5}	Constant temperature (20oC) and pressure (0.55 MPa) on the outer boundary. Maintained until end. 130 W/m2 on the internal boundary.
6 to 20	to 1.728×10^{6}	Power increased to 260 W/m2 on the internal boundary.
20 to 30	to 2.592×10^{6}	Power decreased to 250 W/m2 on the internal boundary.
30 to 60	to 5.184×10^{6}	No changes
60 to 2000	to 1.728×10^{8}	No changes
2000 to 3000	to 2.592×10^{8}	Power shut down to 0 W/m2 on the internal boundary.

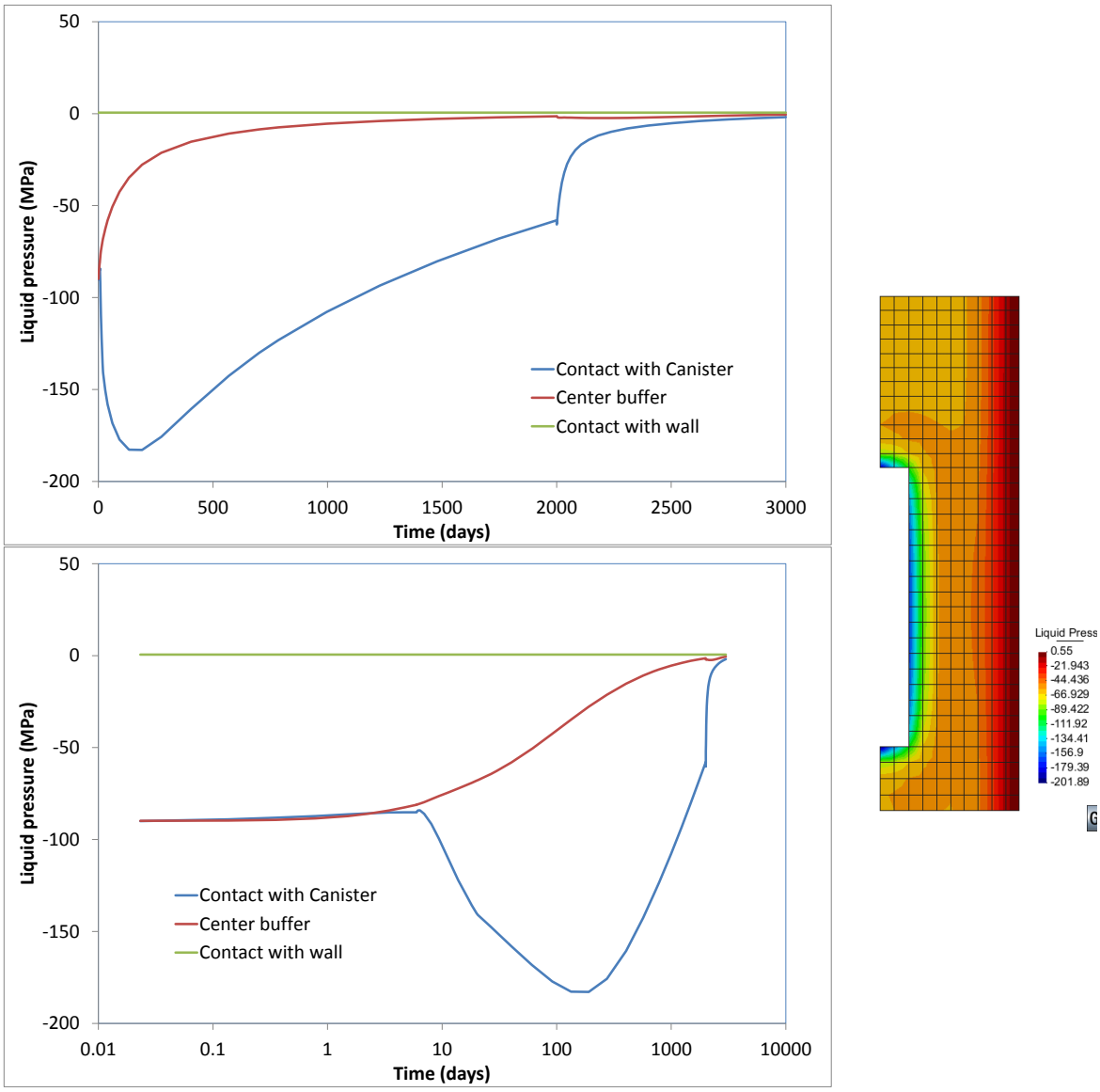
Intervals without changes in boundary conditions are included in this table as these may produce changes on the time step.

Temperature, liquid pressure and mean stress evolutions are included. Heating in various steps takes place and there is a shutdown of heating at 2000 days which causes fast cooling. Liquid pressure shows the effect of heating and associated drying. Mean stress increases because the expansivity of the material which is represented by the BBM model.

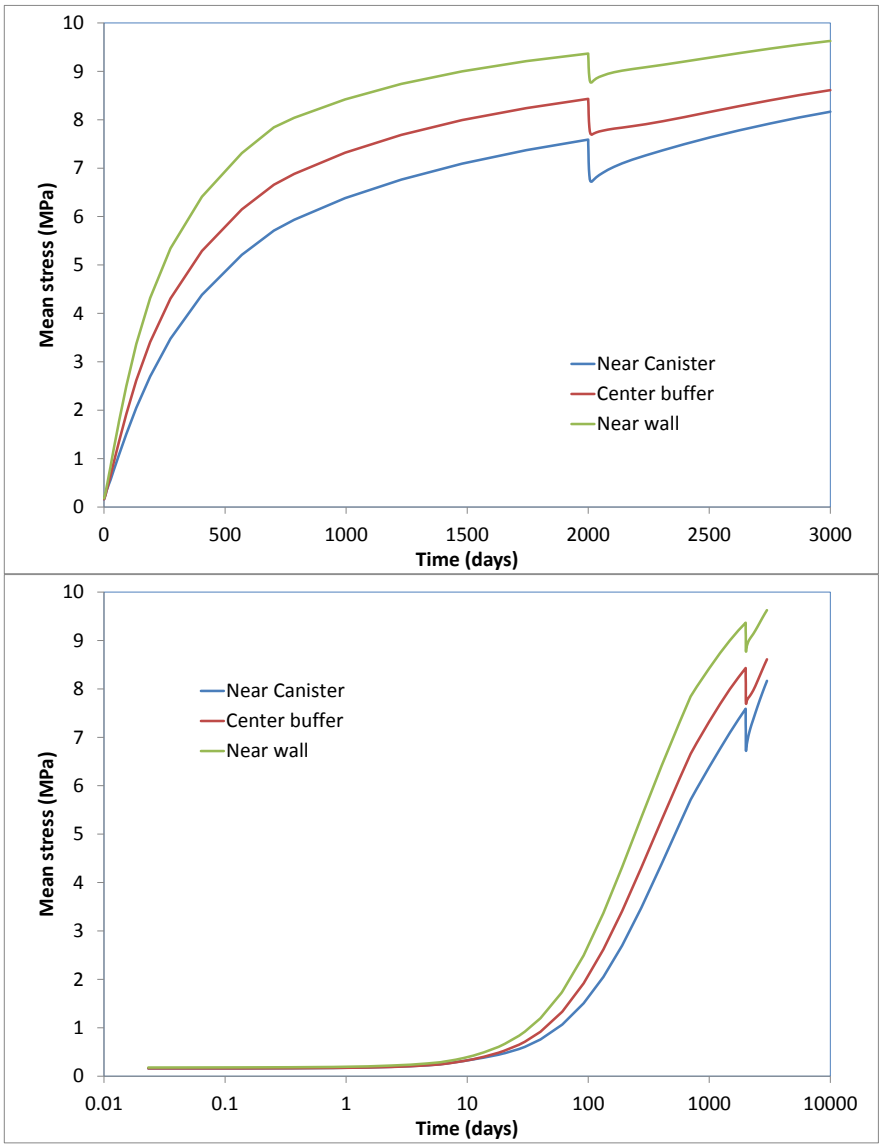


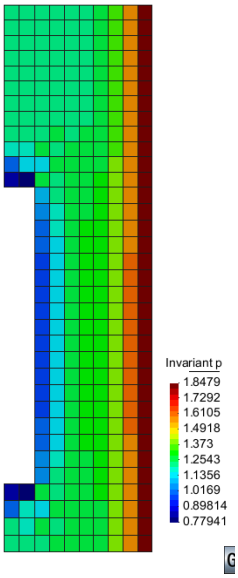


Temperature evolution and power. The point in contact with the canister heats up to somewhat higher than 90oC. The point near the outer surface maintains the 20oC imposed by the atmospheric condition. Time scale is considered linear (above) and logarithmic (center). The figure below corresponds to the variation of the power along time.



Liquid pressure evolution. The point in contact with the canister dries up to a suction that ranges between 150 on 200 MPa. Time scale is considered linear (above) and logarithmic (below).





Mean stress evolution. Mean stress increases during hydration. A contraction is calculated during cooling. Hydration continues after cooling. Time scale is considered linear (above) and logarithmic (below).

2 Time step prediction

A number of options are available in CODE_BRIGHT to perform a time step prediction. The objective of time step prediction is to reduce the numerical error of the calculated results. A consequence of time step prediction must be the reduction of time step rejections. In contrast, a strict time step prediction may produce a large CPU-time needed to finish the calculation. It is desirable to obtain results with low error using an acceptable numerical effort.

A time step prediction scheme has to be chosen for every specific problem. It may depend on accuracy required or desired, non-linearity of the constitutive equations (and this depends on parameters), quality of the mesh, and boundary conditions (instantaneous changes, presence of ramps, non-linear boundary conditions i.e. the ones that depend on the variable at node).

A strict time step prediction scheme may produce good results for a relative simple problem (depending on non-linearity and quality of the mesh) and fail for more complex problems. Failure of time step prediction happens when the estimated errors cannot be limited by time step reduction. In such case, time step predictions become very small and the calculation fails to advance with a reasonable time step to reach the end of the calculation.

The relatively simple model considered here for the runs can be solved with all options for time step prediction discussed in this document (available in CODE_BRIGHT).

The following is a list of options for time step prediction (in CODE_BRIGHT) based on different criteria.

itime	**Description of time step prediction**
0	No time step prediction Maximum number of NR iterations = 10 (*) Maximum variations for time step rejection = 0.1 m, 10 MPa, 0.1 C (*) (*) This is maintained in all cases.
Method based on the number of NR number of iterations	
1	Time step prediction according to an expected target of 4 iterations per time step.
2	Time step prediction according to an expected target of 3 iterations.
3	Time step prediction according to an expected target of 2 iterations
Method based on error estimation of unknowns	
6	A new time step is predicted from the relative error in variables of the previous time step calculation (see below for more detailed description). If the relative error is greater than *dtol* = 0.01, time increment is reduced according to error deviation, otherwise it is increased.
7	The same as 6, but with *dtol* = 0.001
8	The same as 6, but with *dtol* = 0.0001.
9	The same as 6, but with *dtol* = 0.00001.
10	The same as 6, but with *dtol* = 0.000001.
Method based on error estimation combined with second order equation	
16	The same as 6 but second order equation (see below)

17	The same as 7 but second order equation (see below)
18	The same as 8 but second order equation (see below)
19	The same as 9 but second order equation (see below)
Method based on error on stress update	
43	A new time step is predicted from the error in stresses of the previous time step calculation. If the relative error is greater than *dtol* = 0.01, time increment is reduced according to error deviation.
44	The same as 43, but with *dtol* = 0.001
45	The same as 43, but with *dtol* = 0.0001

Description of time step prediction options in CODE_BRIGHT

Value 0

No time step prediction is performed.

Time step is controlled by the user given values according to the time interval definition window. An upper bound of time step is considered. Time step rejections (and subsequent reductions) can occur if convergence is not achieved or other reasons.

Convergence implies that time step will be increased by a factor of 1.4 regardless of the number of iterations or evolution of errors. Maximum number of iterations reached implies time step reduction by a factor of 0.5. On the other hand, if large variations of displacements, pressures or temperatures occur during a NR iteration, time step is reduced immediately simply by scaling, and calculations start again for the current time step.

The values considered in the calculations are:
Maximum number of NR iterations = 10
Maximum variation, for time step rejection, of displacement, pressure and temperature, = 0.1 m, 10 MPa, 0.1 C, respectively. For instance, if temperature variation is 0.5, time step is reduced by a factor of 1/5.

Time step rejections are not desirable, but can occur. This is maintained in all cases.

Values of 1, 2, 3

The number of Newton Raphson iterations is used to estimate the value of the time step that will be used after convergence for the next time step calculation. There are three possibilities in this case according to 4, 3 or 2 Newton Raphson iterations.

Time step control value (ITIME) = 1 $\quad f = \left(\frac{4}{iter}\right)^{0.25} \geq 0.5$

Time step control value (ITIME) = 2 $\quad f = \left(\frac{3}{iter}\right)^{0.25} \geq 0.5$

Time step control value (ITIME) = 3 $\qquad f = \left(\frac{2}{iter} \right)^{0.25} \geq 0.5$

The value of *f* has an upper bound of 1.4. Note that *f* = 1 when the target of number of iterations is obtained and this implies same time step.

If the maximum time step prescribed manually (DTIMEC) is achieved, time step will not increase above this value regardless of what the formula indicates.

Values of 6, 7, 8, 9, 10

An estimation of error (for displacements, pressures and temperatures) is used to predict time step. Time step is predicted with the factor *f* which is calculated with:

$$f = 0.8 \left(\frac{DTOL}{error} \right)^{0.5} \qquad \text{with } 0.1 \leq f \leq 1.4$$

The variable *error* is calculated using an error estimator based on second order prediction. An upper and lower bound for *f* are considered.

The value of *DTOL* has the following values depending on the option chosen:

6 *DTOL* = 0.01 (not used in this study)
7 *DTOL* = 0.001
8 *DTOL* = 0.0001
9 *DTOL* = 0.00001
10 *DTOL* = 0.000001 (used in this study to obtain a reference solution).

If the maximum time step prescribed manually (DTIMEC) is achieved, time step will not increase furthermore.

Values of 16, 17, 18, 19

Same as 6,7,8,9 but second order approximation of conservation equations is used. This is based on the following equations (for implicit scheme):

$$\left(\frac{2\left(\mathbf{m}(\mathbf{x}_n) - \mathbf{m}(\mathbf{x}_{n-1})\right) - h\dot{\mathbf{m}}(\mathbf{x}_{n-1})}{h} \right) + \left[\mathbf{K}(\mathbf{x}_n)\right]\mathbf{x}_n = \mathbf{F}_n$$

This is a modification of the usual approach in CODE_BRIGHT which can be written in the following compact way:

$$\left(\frac{\mathbf{m}(\hat{\mathbf{x}}_n) - \mathbf{m}(\mathbf{x}_{n-1})}{h} \right) + \left[\mathbf{K}(\hat{\mathbf{x}}_n)\right]\hat{\mathbf{x}}_n = \mathbf{F}_n$$

If the maximum time step prescribed manually (DTIMEC) is achieved, time step will not increase furthermore.

Values of 43, 44, 45

An estimation of error (stresses) is used to predict time step. Time step is predicted with the factor *f* which is calculated with:

$$f = 0.8\left(\frac{DTOL}{error}\right)^{0.5} \qquad \text{with } 0.1 \le f \le 1.4$$

The variable *error* is calculated using an error estimator for stresses. The variable *f* is the factor for time step reduction. An upper and lower bound for *f* are considered.

The value of *DTOL* has the following values depending on the option chosen:

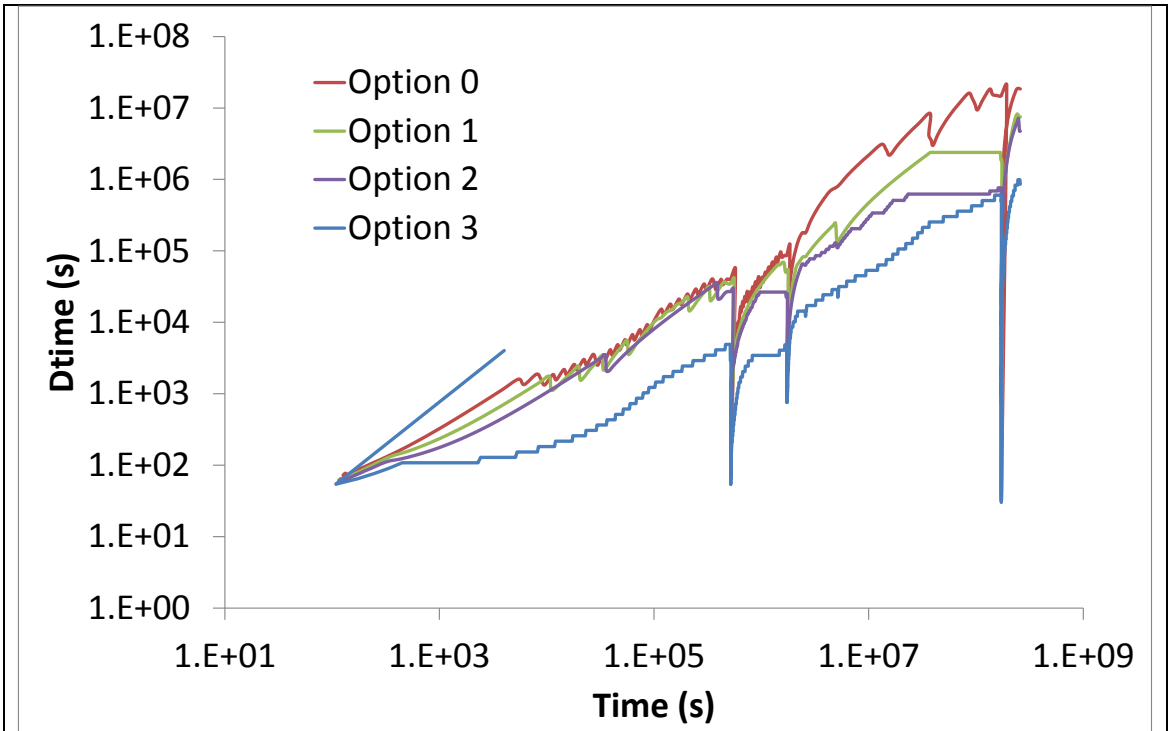
43 *DTOL* = 0.001
44 *DTOL* = 0.0001
45 *DTOL* = 0.00001

If the maximum time step prescribed manually (DTIMEC) is achieved, time step will not increase furthermore.

3. Time step evolution during model run

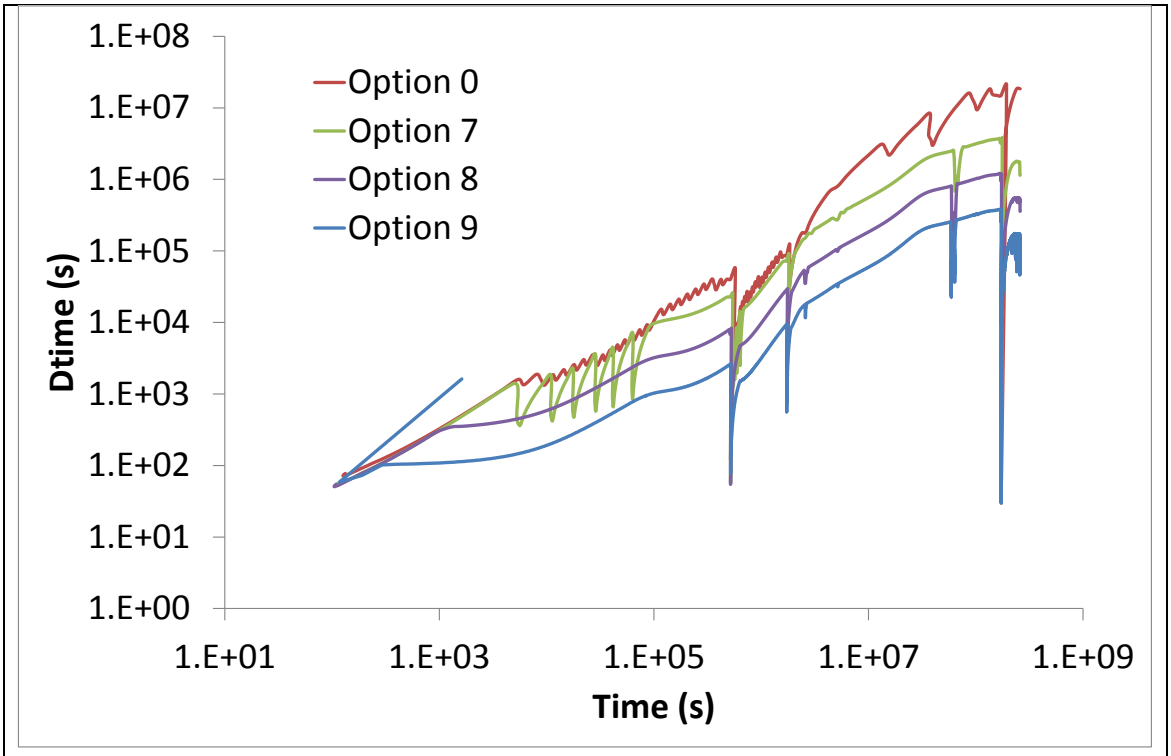
A typical plot of time step evolution has been prepared for each run as a function of time. Some of the time step reductions correspond to changes in boundary conditions:

Time days	*Time seconds*	*Boundary condition changes*
0 to 6	0 to 5.184×10^{5}	Constant temperature (20oC) and pressure (0.55 MPa) on the outer boundary. Maintained until end. 130 W/m2 on the internal boundary.
to 20	to 1.728×10^{6}	260 W/m2 on the internal boundary.
to 30	to 2.592×10^{6}	250 W/m2 on the internal boundary.
to 60	to 5.184×10^{6}	No change
to 2000	to 1.728×10^{8}	No change
to 3000	to 2.592×10^{8}	0 W/m2 on the internal boundary

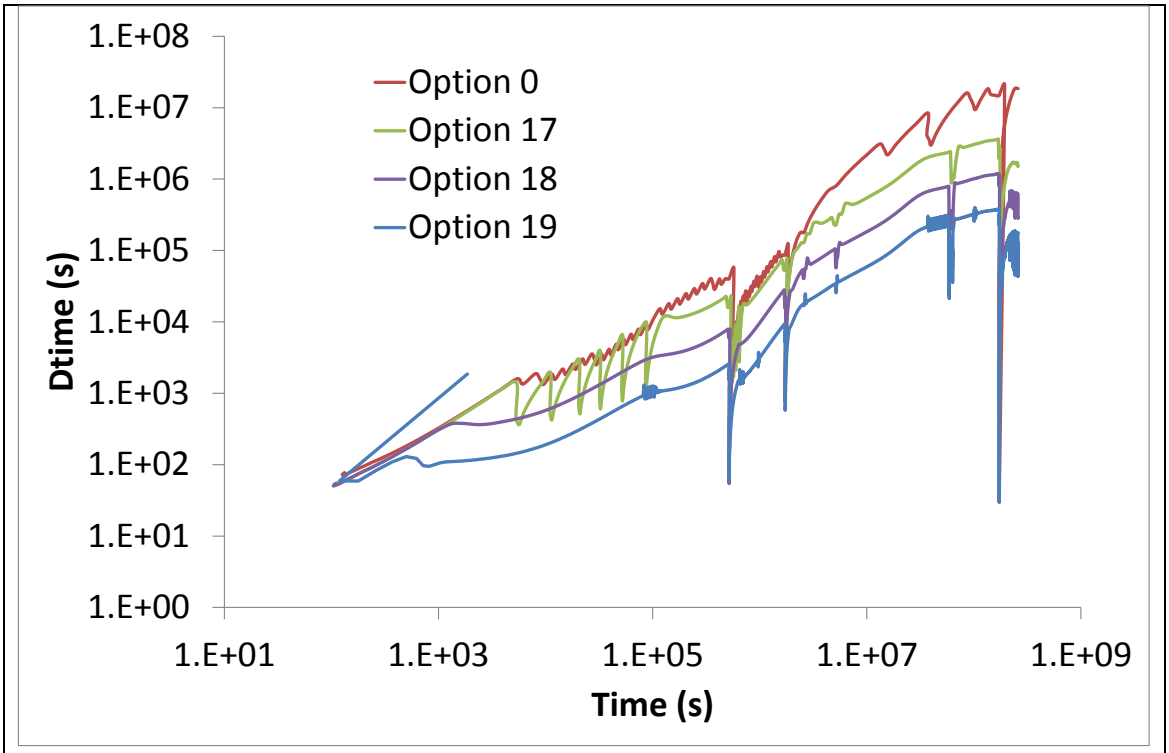


Time step evolution for option (itime) = 0. No time step prediction is done, only time step rejection by failure to converge and subsequent reduction. User defined time step control is not given, hence time step can grow as much as possible. But 128 time step rejections and immediate reductions encountered due to convergence problems or too large variations of variables (displacement, pressure or temperature). In conclusion, time step evolution is only controlled by NR convergence difficulties.

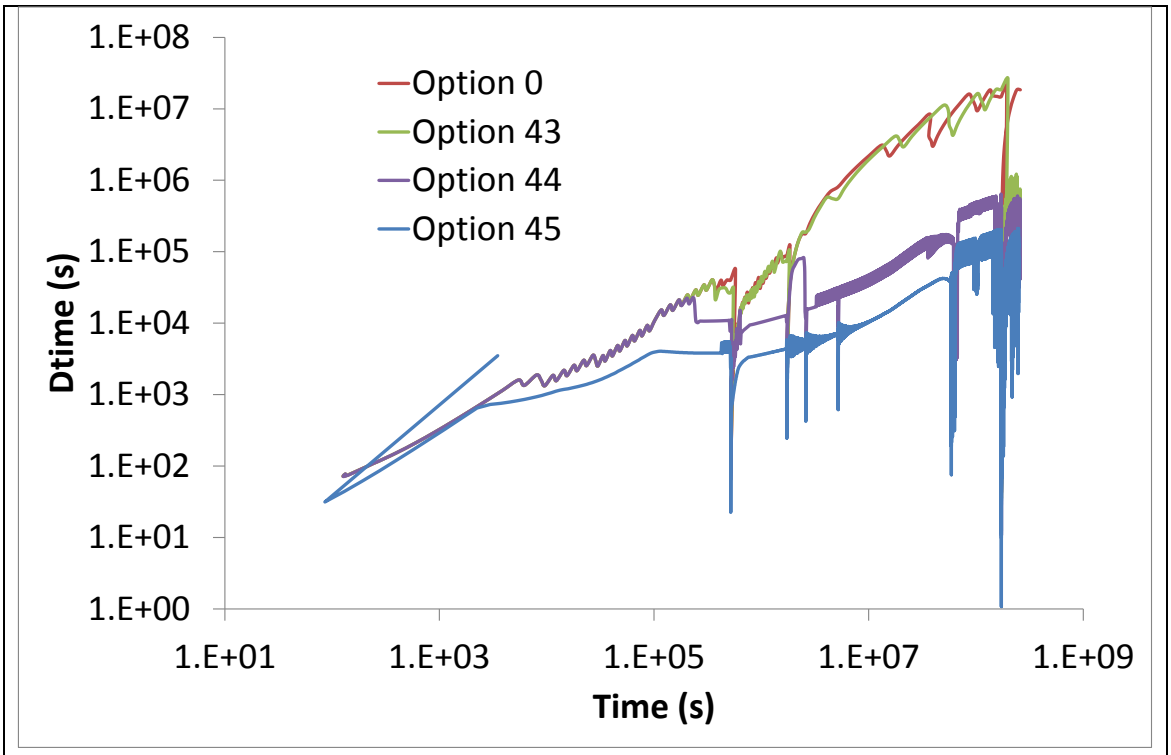
Time step for itime =1,2 and 3		
Itime= 0	128 time step rejections	327 time steps
Itime = 1	37 time step rejections	483 time steps
Itime = 2	21 time step rejections	762 time steps
Itime = 3	13 time step rejection	3261 time steps



Time step for itime =7, 8 and 9		
Itime = 7	41 time step rejections	569 time steps
Itime = 8	15 time step rejections	1362 time steps
Itime = 9	10 time step rejections	4203 time steps



Time step for itime =17, 18 and 19		
Itime = 17	40 time step rejections	570 time steps
Itime = 18	15 time step rejections	1376 time steps
Itime = 19	10 time step rejections	4226 time steps



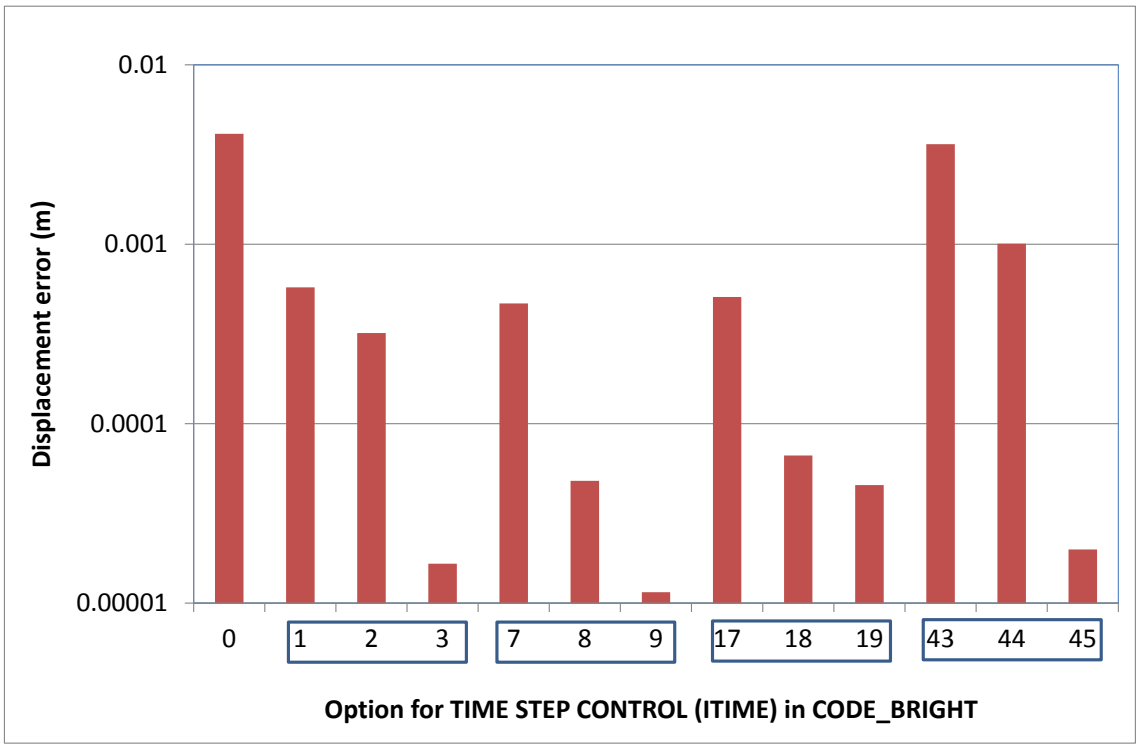
Time step for itime = 43, 44 and 45		
Itime = 43	83 time step rejections	580 time steps
Itime = 44	45 time step rejections	2746 time steps
Itime = 45	12 time step rejections	8491 time steps

4 Calculated error and computational cost

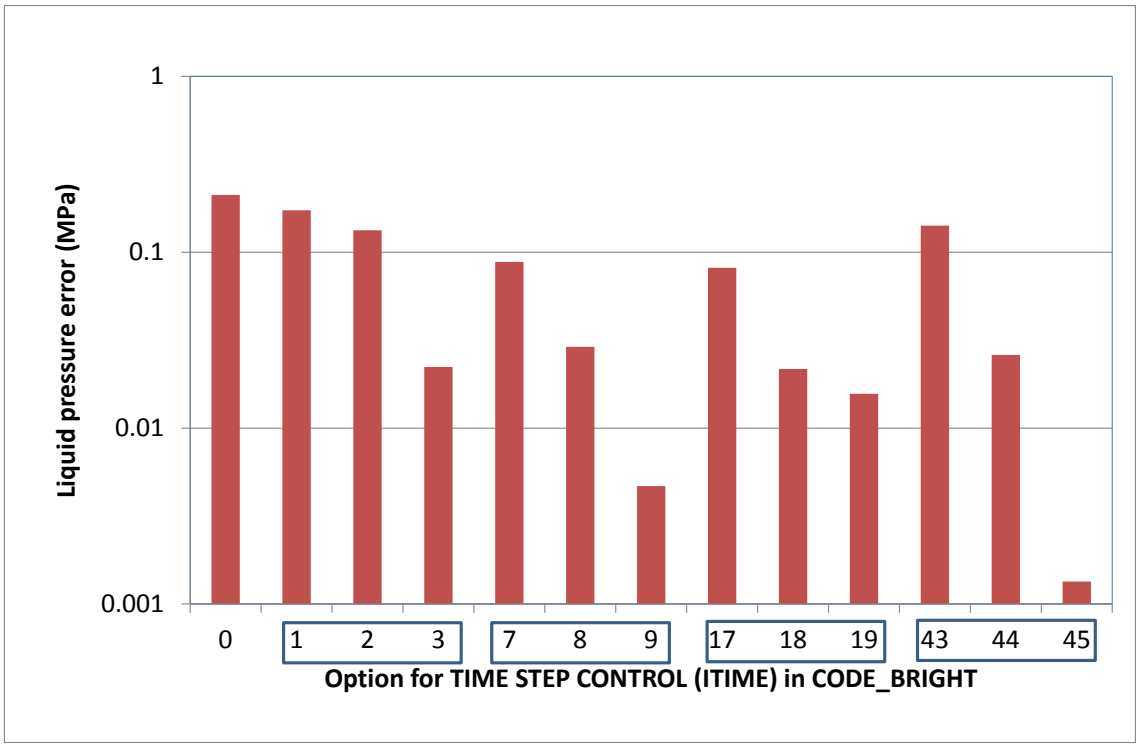
A reference case that uses very small time steps is used to determine the error of each run. This very small time step case uses one Newton Raphson iteration for every time step during the calculation as the time step is so small that corrections at every time steps are smaller than tolerances. This is achieved with *DTOL* = 0.000001. Errors are calculated as difference between calculated results at the final time. This can be done for unknowns (displacement, pressure, temperature) or for any other variable. The maximum variable error for all nodes is considered for each variable.

CPU time is normalized with respect to the CPU time required to solve case "0". The maximum value is 9 times for one of the prediction schemes. CPU time becomes larger mainly because time step is smaller. Smaller time steps imply lower number of NR iterations. The fact that lower NR iterations are used does not compensate the effect of more time steps. Hence, smaller time steps always imply more CPU time.

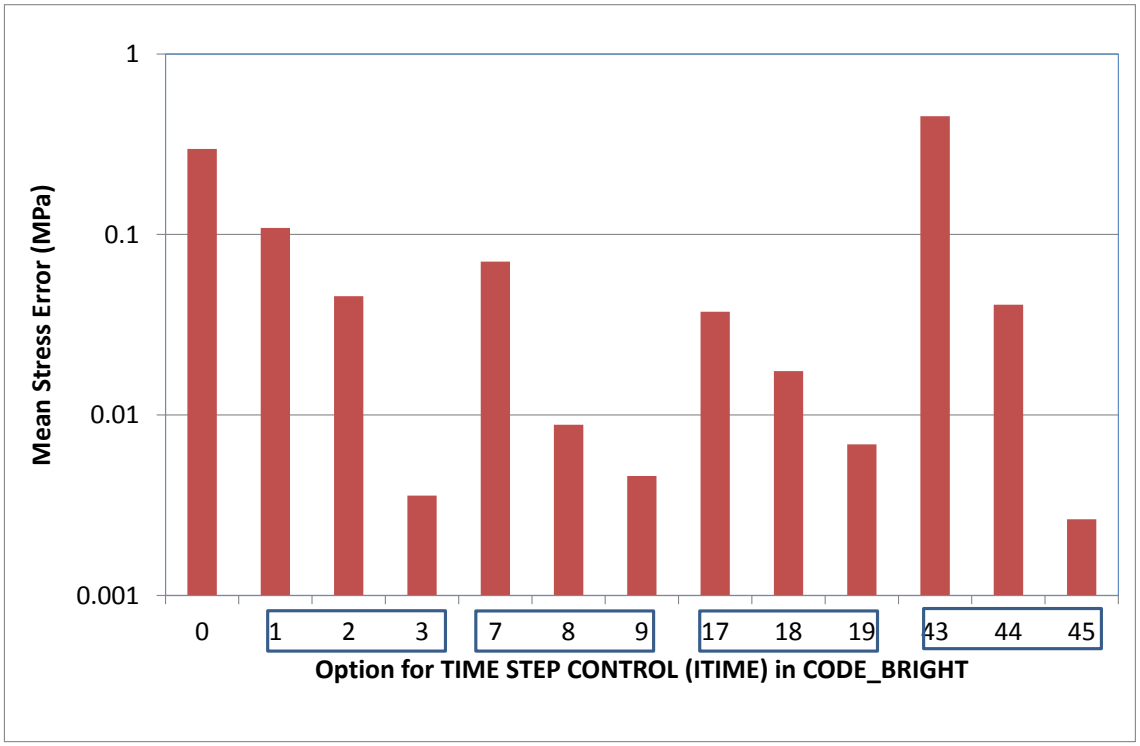
The number of NR iterations ranges between 1 and 3 in average. When the average is 1, it means that all time steps require one NR iteration.



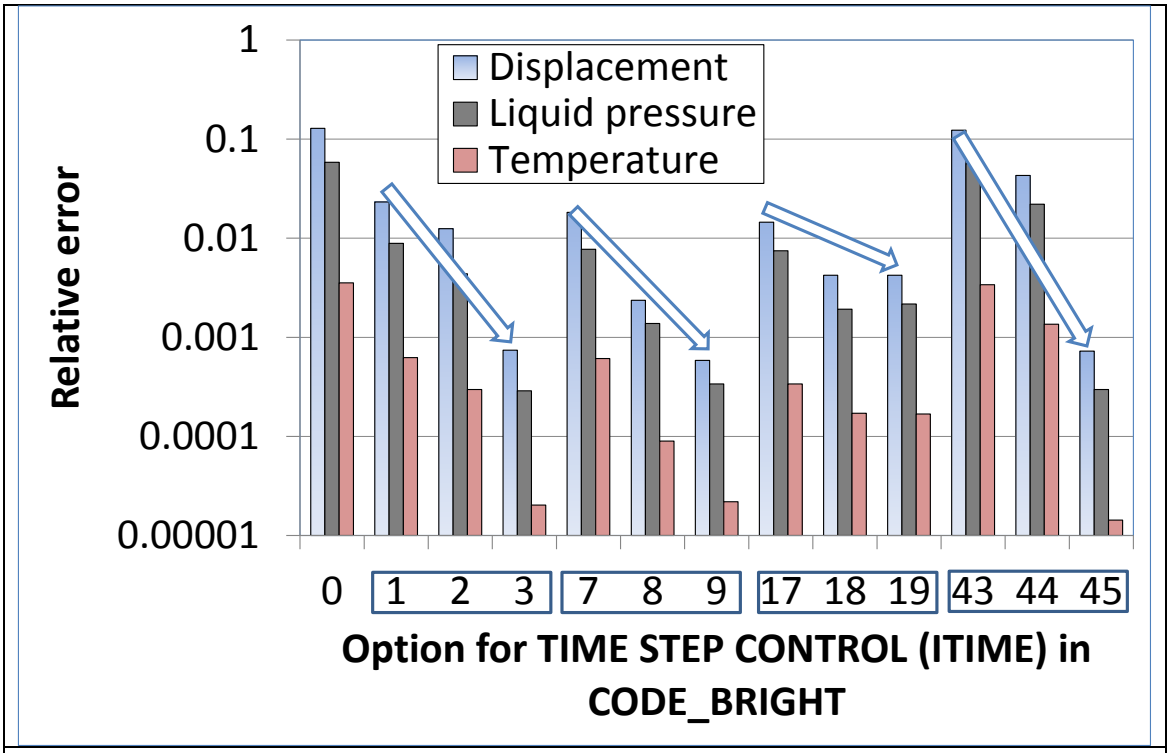
Absolute error for displacement at the end of model calculation (3000 days) for the node that has the maximum error.



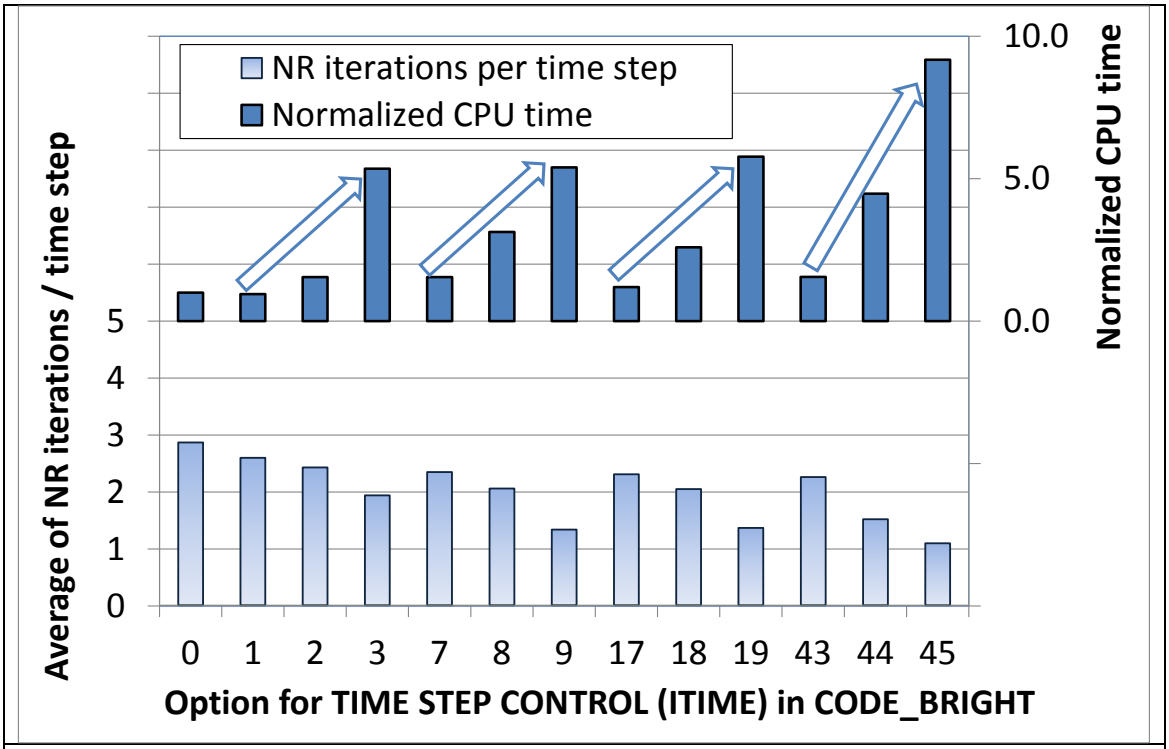
Absolute error for liquid pressure at the end of model calculation (3000 days) for the node that has the maximum error.



Absolute error for mean stress at the end of model calculation (3000 days) for the node that has the maximum error.



Relative error for displacements, liquid pressures and temperatures calculated using resultsat 60 days.



Normalized CPU time and Average number of NR iterations for model runs with different options for time step predictions.
CPU time increases when "time step control" method is stricter because time steps are smaller. This is compensated by the reduction on the number on NR iterations.

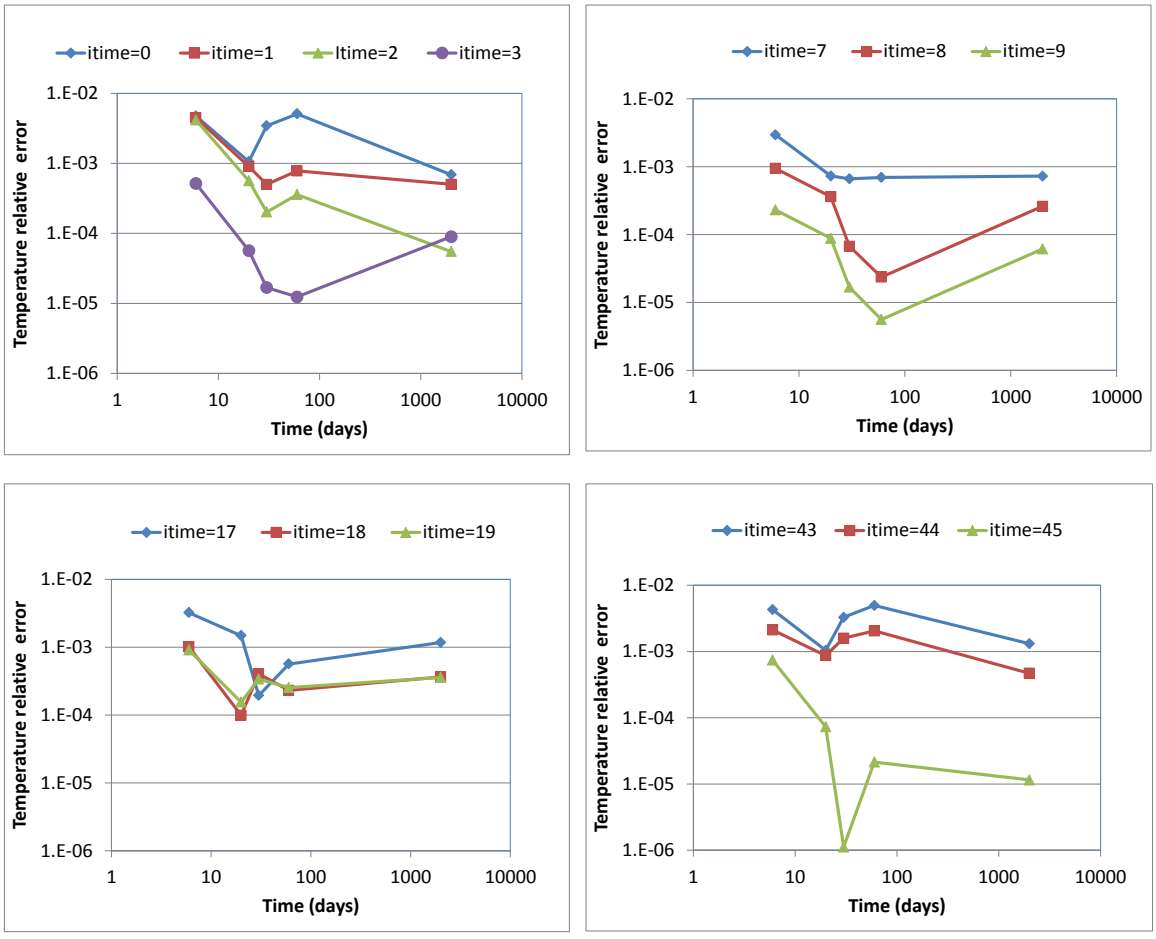
Option 2 leads to 2.5 NR iterations per time step. CPU time is moderately bigger than the reference case Option 0. Error in variables is approximately 10 times lower than the reference case Option 0. Hence, this is an interesting option.

Option 8 leads to 2 NR iterations per time step. CPU time is 3 times the reference case. Error in variables is about 20-30 times lower than the reference case Option 0. This is an interesting option provided that an increase of CPU time is accepted.

Evolution of error during calculations

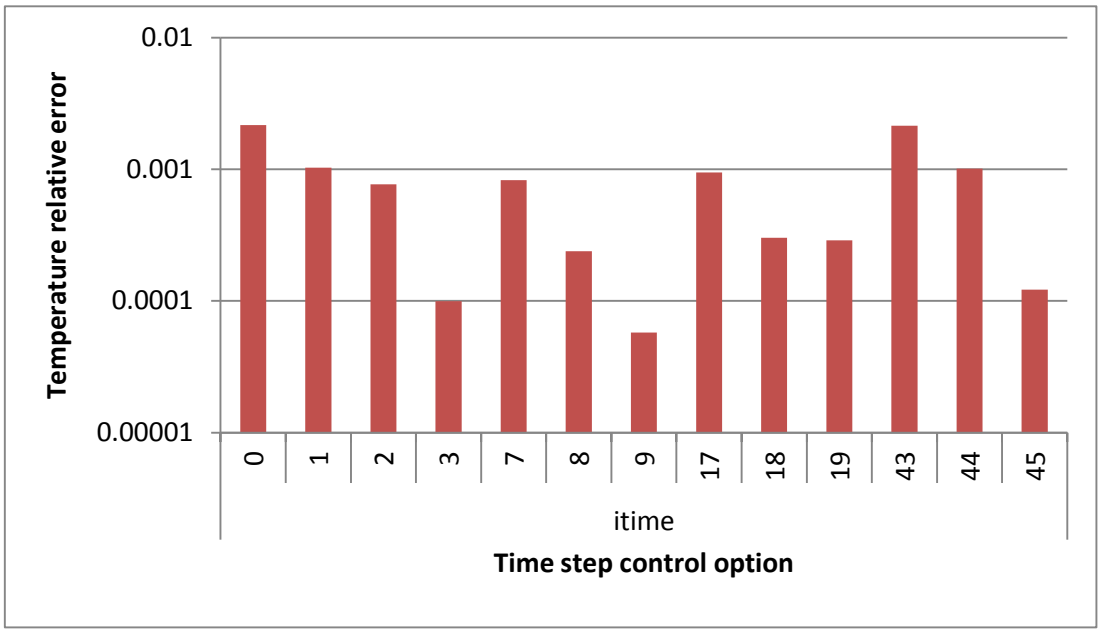
Final temperature in the calculation is constant and therefore it is not possible to calculate errors at 3000 days. For this reason this has not been included in the previous section. Instead, a point in the hottest zone on the surface where the heat inflows, has been used to calculate the error at certain times. Intermediate points (the beginning-end of intervals) are adequate because these are exact times where the calculation gives output values.

The following figures show the relative error for temperature in a point on the hot boundary.



Relative error in temperature at hottest point during model evolution

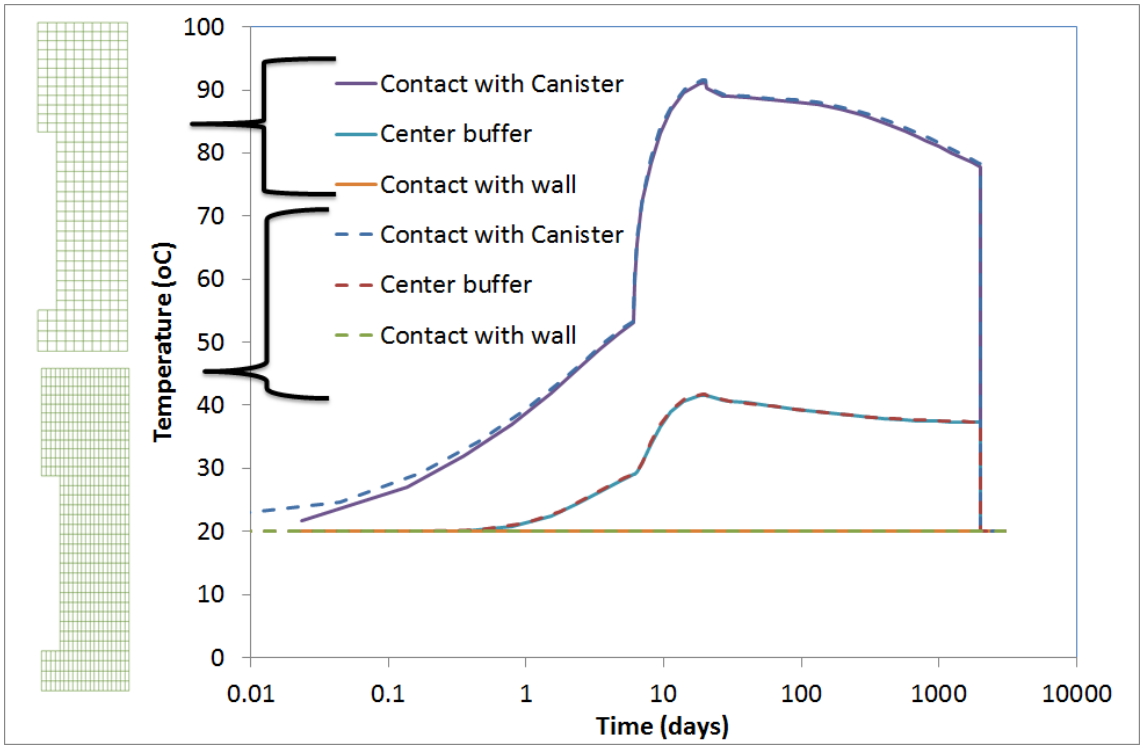
From error evolution it is observed that relative error may change during the evolution of the coupled problem. These errors can be average over time to obtain a plot similar to what has been obtained for other variables.



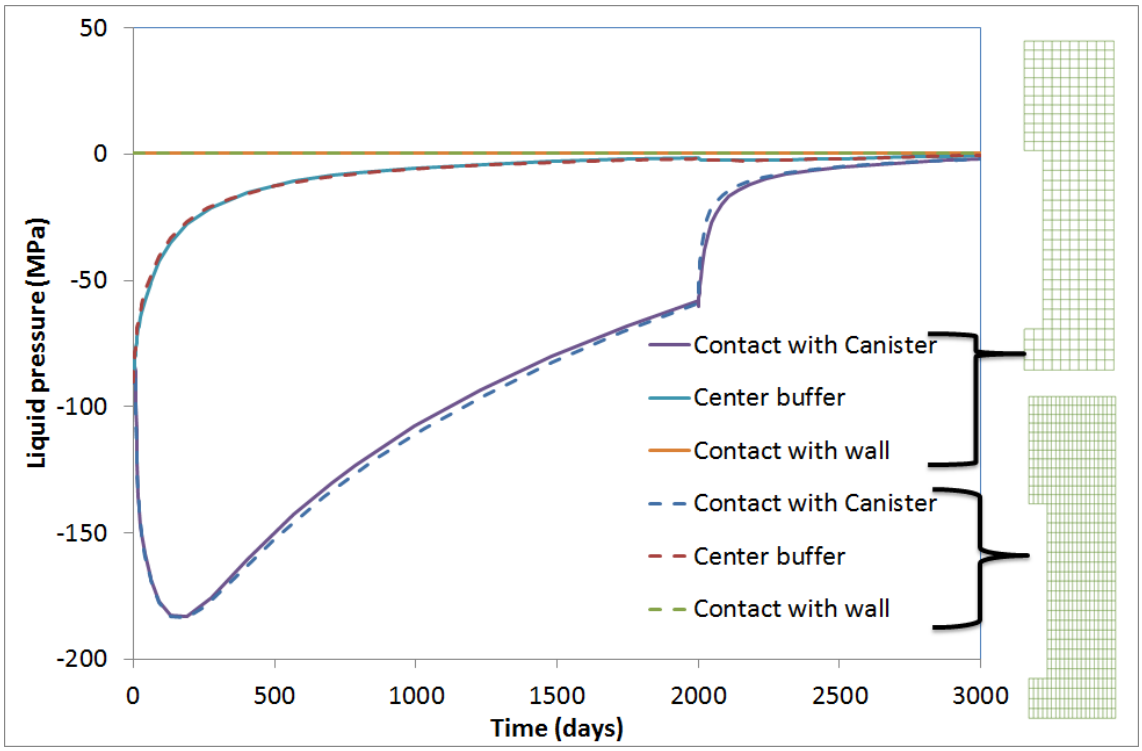
Temperature relative error calculated in a point (hottest zone) and averaged for various times

5 Effect of mesh size

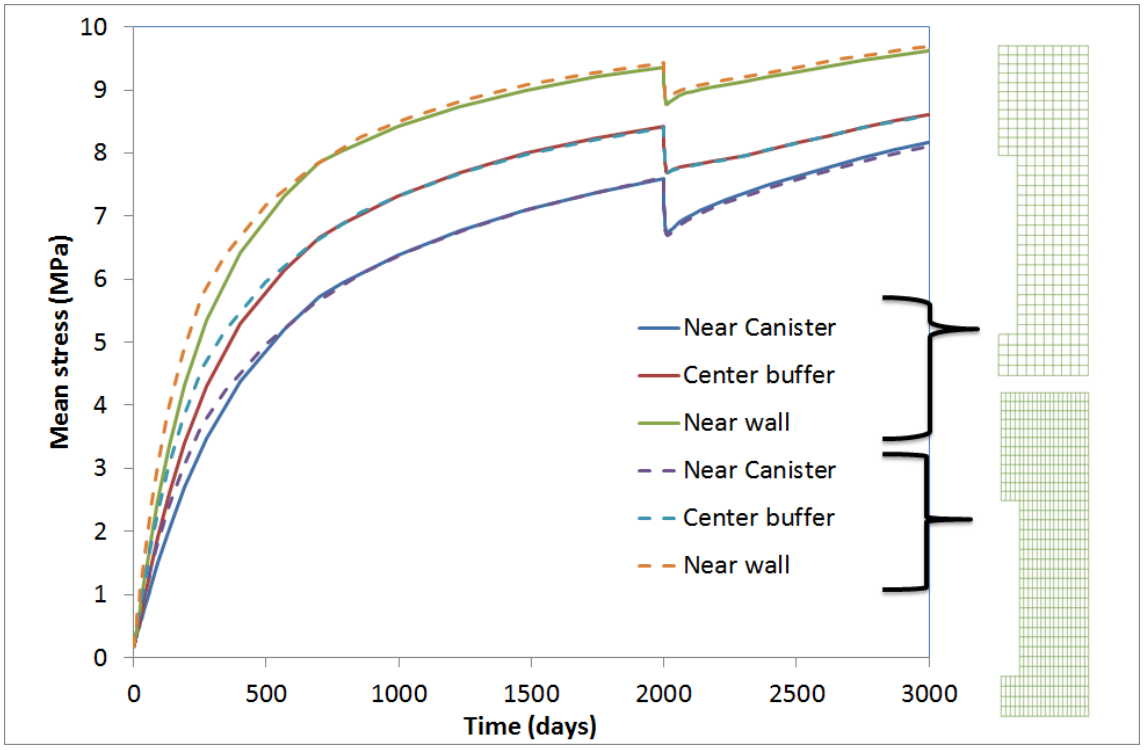
The results shown above are obtained with the same tendencies if another mehs is used. Mesh size effect can be illustrated by comparing liquid pressure evolution for example as it is the variable with largest error. With a mesh half size, the results are practically identical.



Comparison of temperature evolution at selected points for two different meshes.

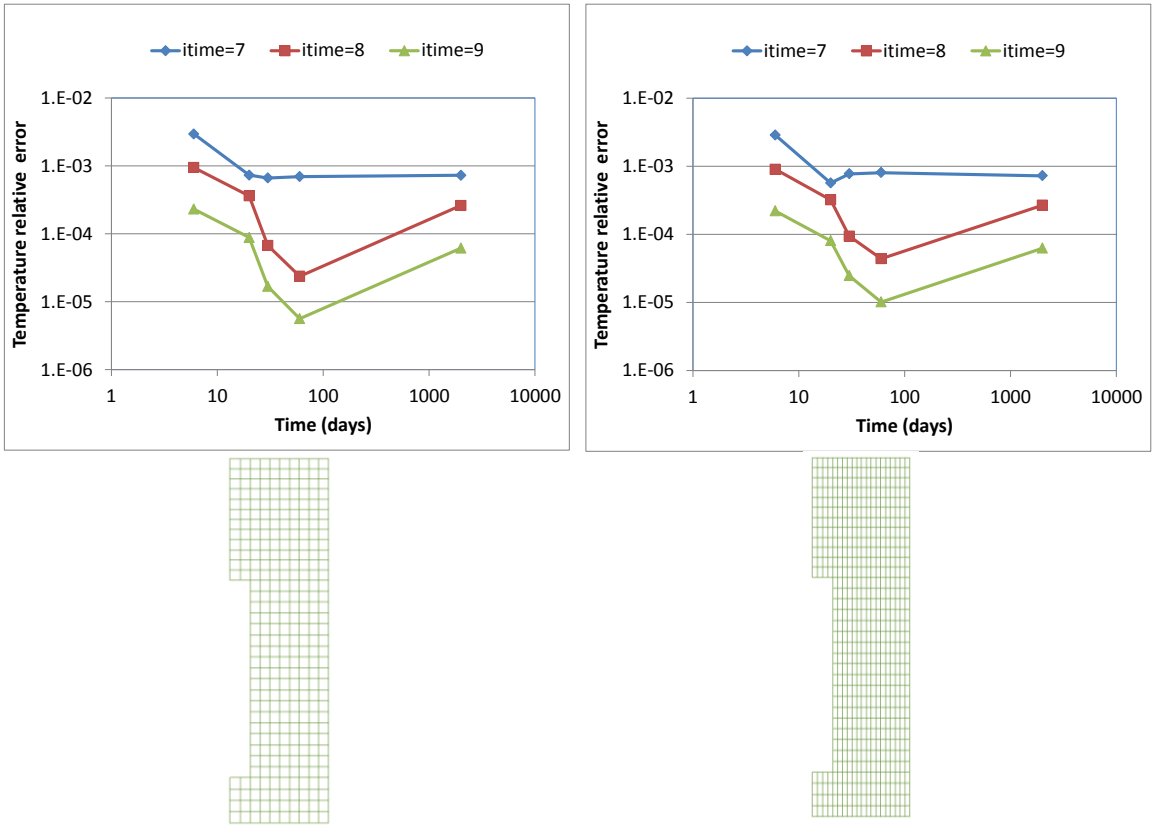


Comparison of liquid pressure evolution at selected points for two different meshes.



Comparison of mean stress evolution at selected points for two different meshes.

Each mesh defines a different problem. The errors are calculated by comparison of results obtained with the same mesh. So, the effect of time step control is analysed for each mesh giving the same error variations.

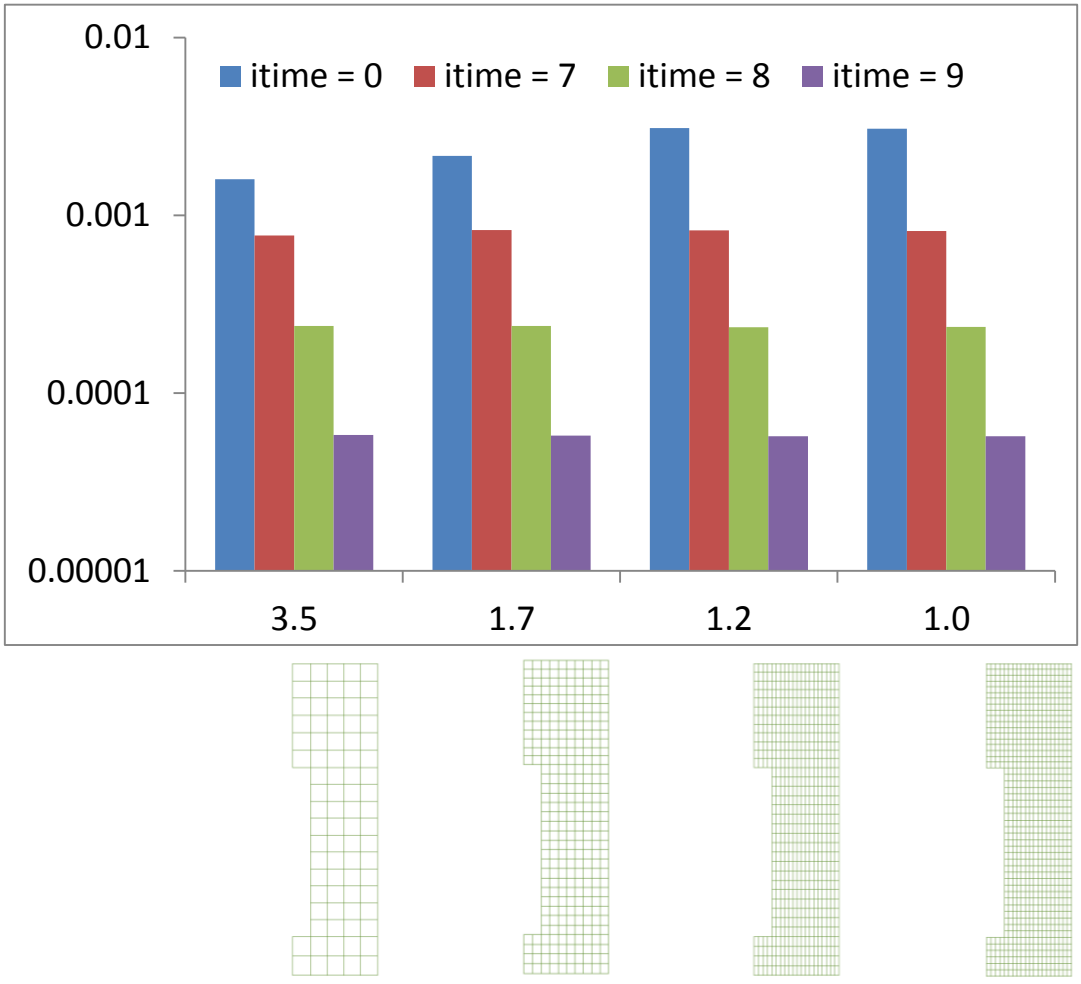


Relative error in temperature for time step control options 7, 8 and 9. Left with squared elements, right for the rectangular elements (half size of the squared). Each mesh has a reference solution.

Combined effect of time step and mesh

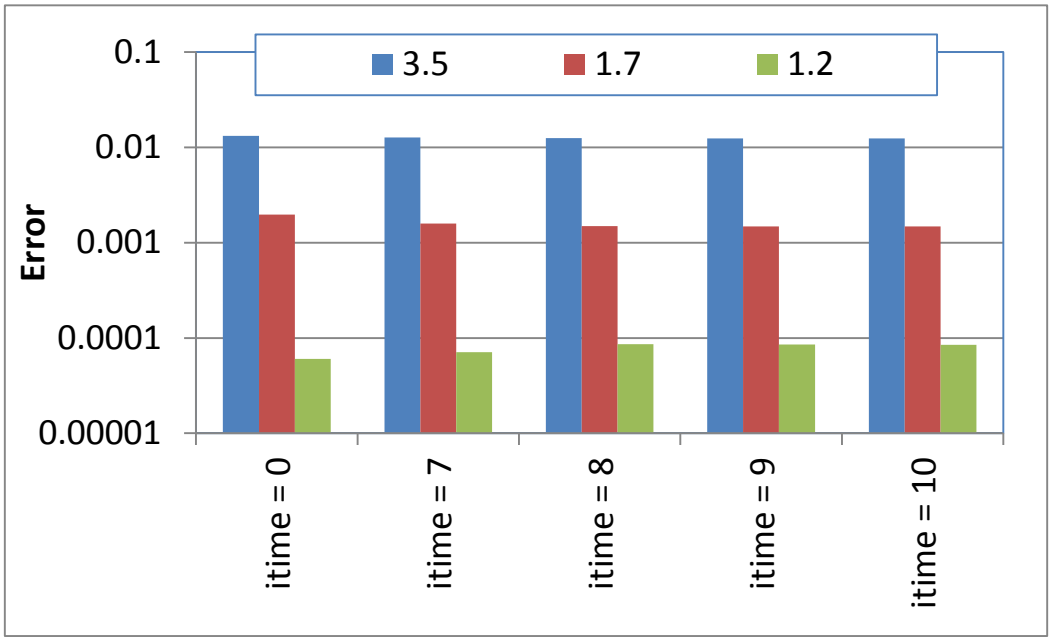
To investigate the effect of time step control and mesh size, calculations with different mesh sizes and time step control system have been carried out. 4 meshes and 5 time step control options have been considered.

Firstly, the effect of time step control for different mesh sizes is analysed. Each mesh is considered to do the study of time step control. The results to compare the error are for each mesh, the ones obtained with itime = 10. For each mesh size, there is a different reference model to calculate the error. In other words, given a mesh the systematic study of time step control gives practically the same error variation.



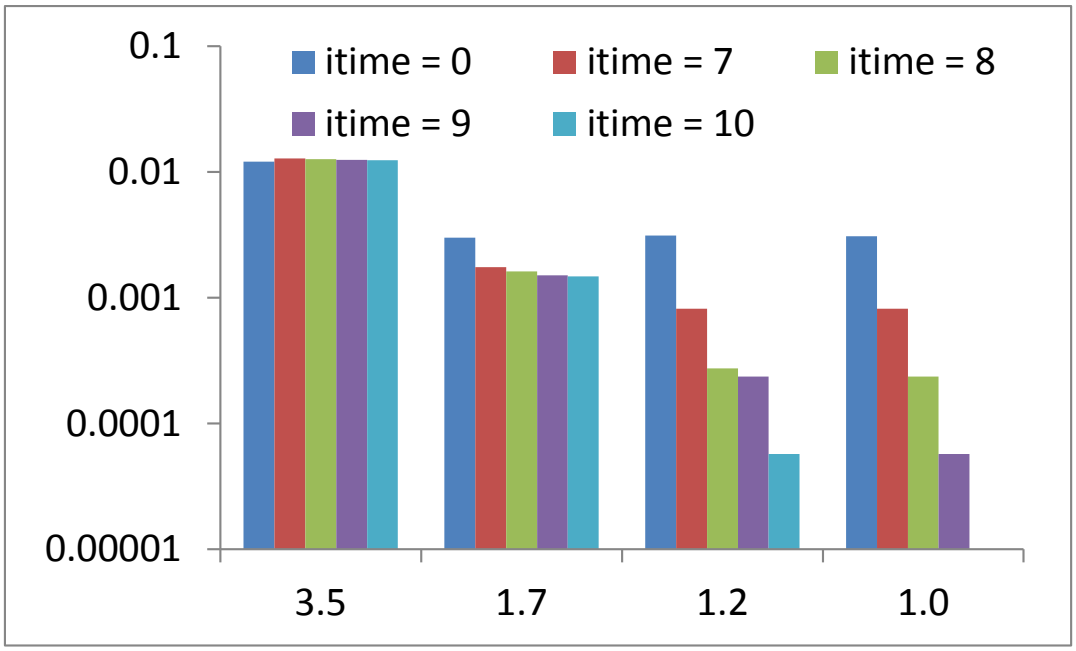
Effect of mesh size on the reduction of error caused by different time step control system. For each mesh (defined by the normalized element size), time step control with smaller error tolerance, reduces in the same way the error.

Secondly, the effect of mesh is analysed. For each time step control system, the effect of the mesh is analysed. Similar error reduction is obtained.



Effect of time step control system on the reduction of error caused by different mesh sizes. For each time step control, smaller mesh reduces the error in the same way.

Finally, the combined effect of mesh and time step control is analysed. The results for different mesh size and time step control method are compares with the case of itime=10 and mesh size equal to 1. This reference case is supposed to be the case with less error of all calculations. The plot indicates that if the mesh is large (3.5), improving the time step method (i.e. reducing time step) does not improve the solution.



Error calculated with respect to one single case (itime=10 and mesh size = 1).

6 Time step control used without time step rejections

The different options explained here have been used in combination with time step rejection options available in CODE_BRIGHT. As indicated above, time step rejection has been done according to the actions described below.

Maximum number of iterations reached implies time step reduction by a factor of 0.5. On the other hand, if large variations of displacements, pressures or temperatures occur during a NR iteration, time step is reduced immediately simply by scaling, and calculations start again for the current time step.

The values considered in the calculations are:

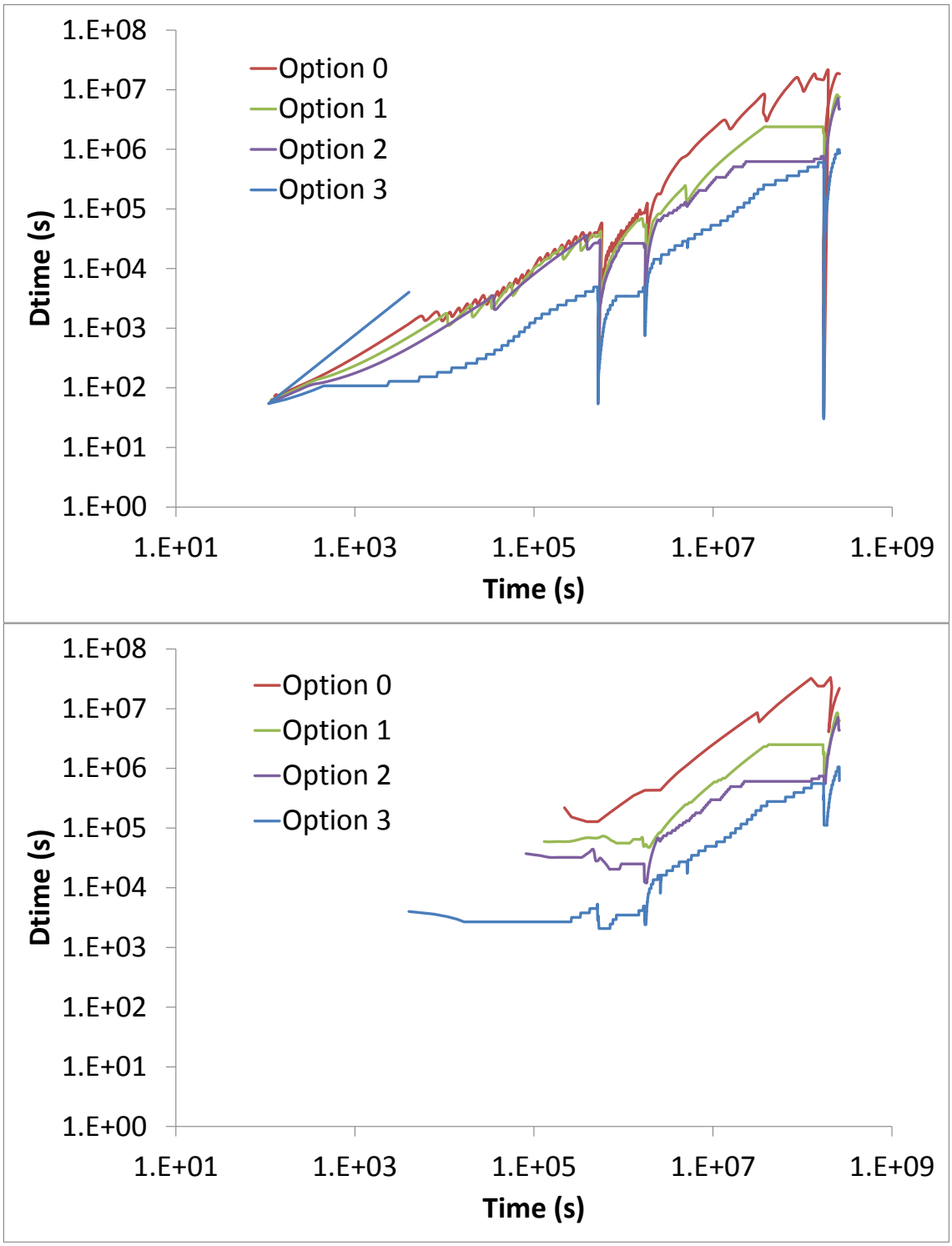
Maximum number of NR iterations = 10

Maximum variation, for time step rejection, of displacement, pressure and temperature, = 0.1 m, 10 MPa, 0.1 C, respectively. For instance, if temperature variation is 0.5, time step is reduced by a factor of 1/5. In addition, time step can be reduced if correction increase or convergence is slow.

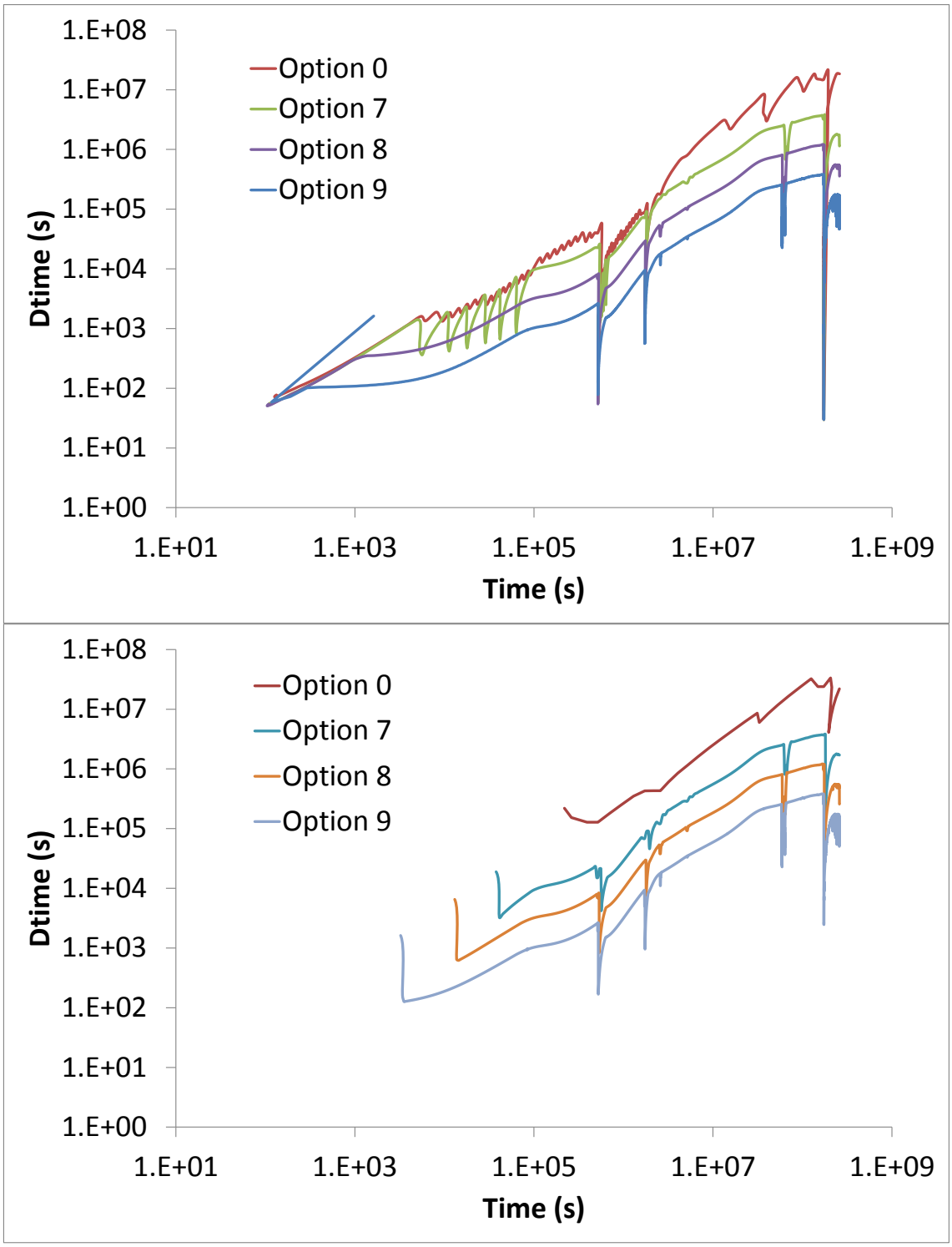
In this section, the number of time step rejections is reduced as much as possible. This is based on the following objectives:

- To reduce the risk of non-convergence when time step rejections and subsequent reductions becomes endless and time step reduces a lot thus stopping the run.
- To reduce the risk of too small time steps after boundary condition change which may lead to large variations of variables.
- To reduce the risk of out of scale results obtained with very small time steps.
- To avoid CPU time waste as rejection and reduction imply waste of CPU time.

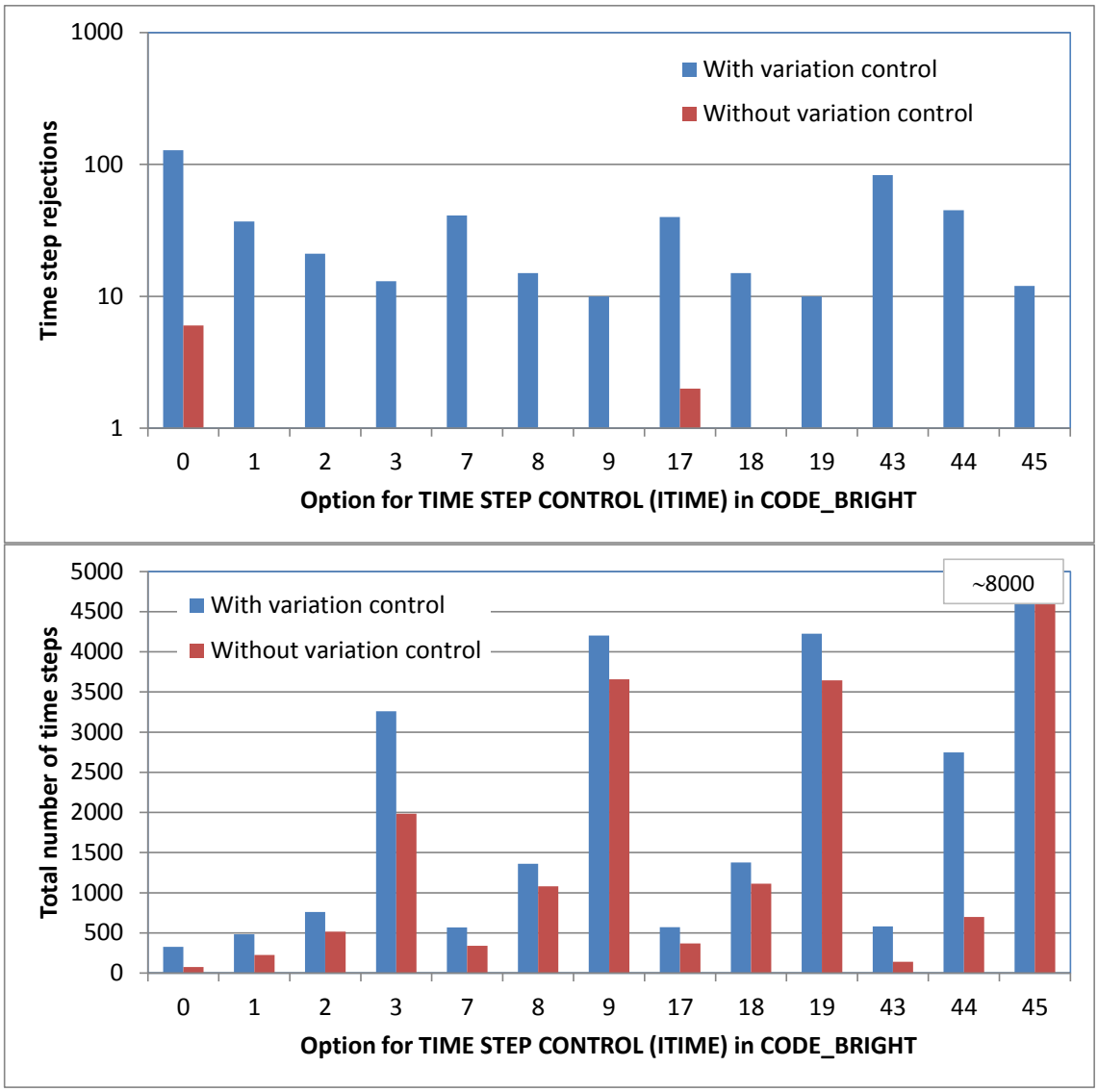
To reduce rejections, the control of variations of variables has been removed by setting large values on the corresponding tolerances for variation. So, instead of the above mentioned values, 0.1 m, 10 MPa, 0.1 C, a large value is input. The maximum number of NR iterations is maintained to 10 which is considered sufficiently large so it is not expected to play a significant role when time step is controlled automatically.



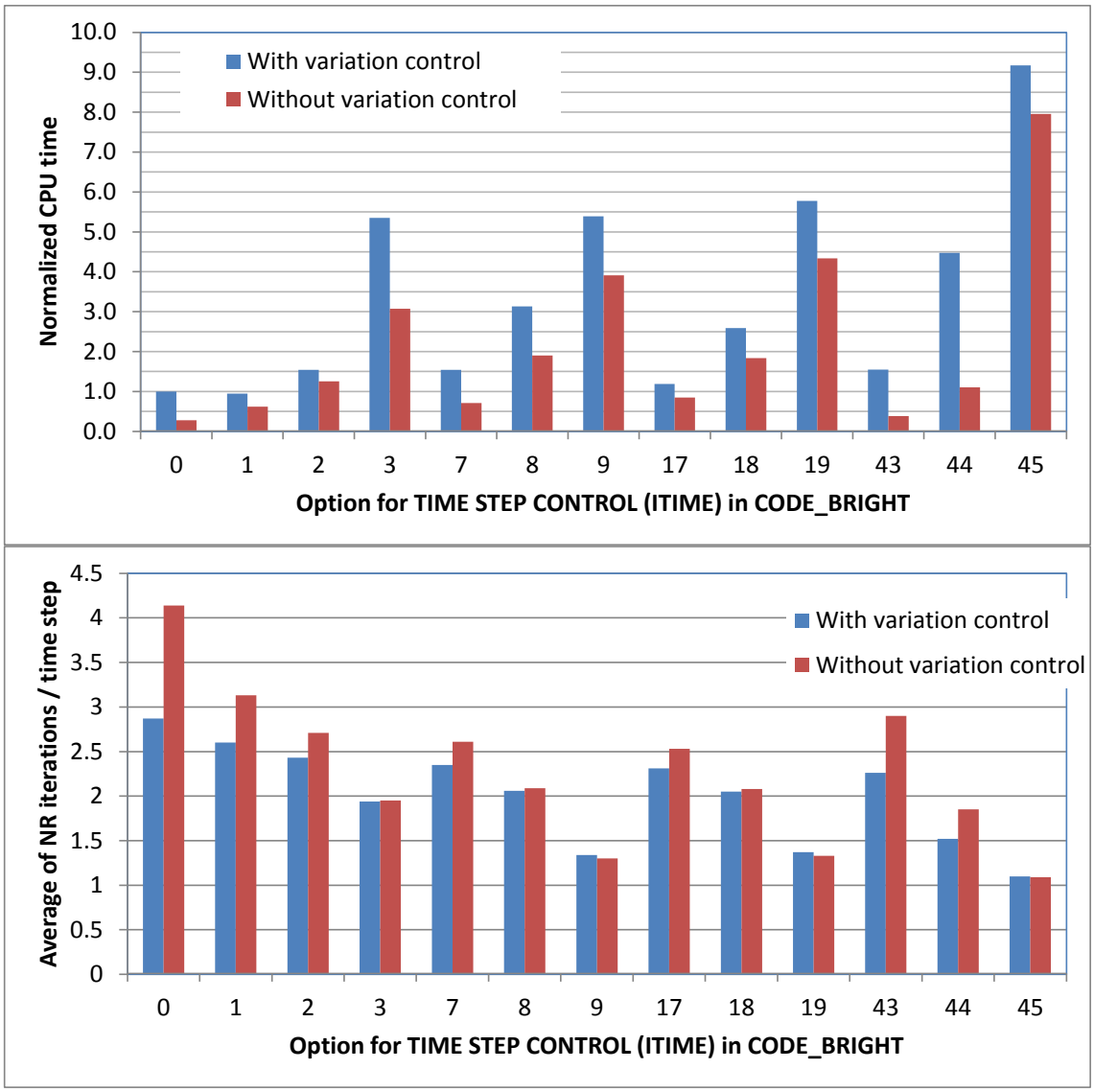
Evolution of time step during model run. The model uses (above) or not uses (below) the time step rejection method based large variations of calculated variables.



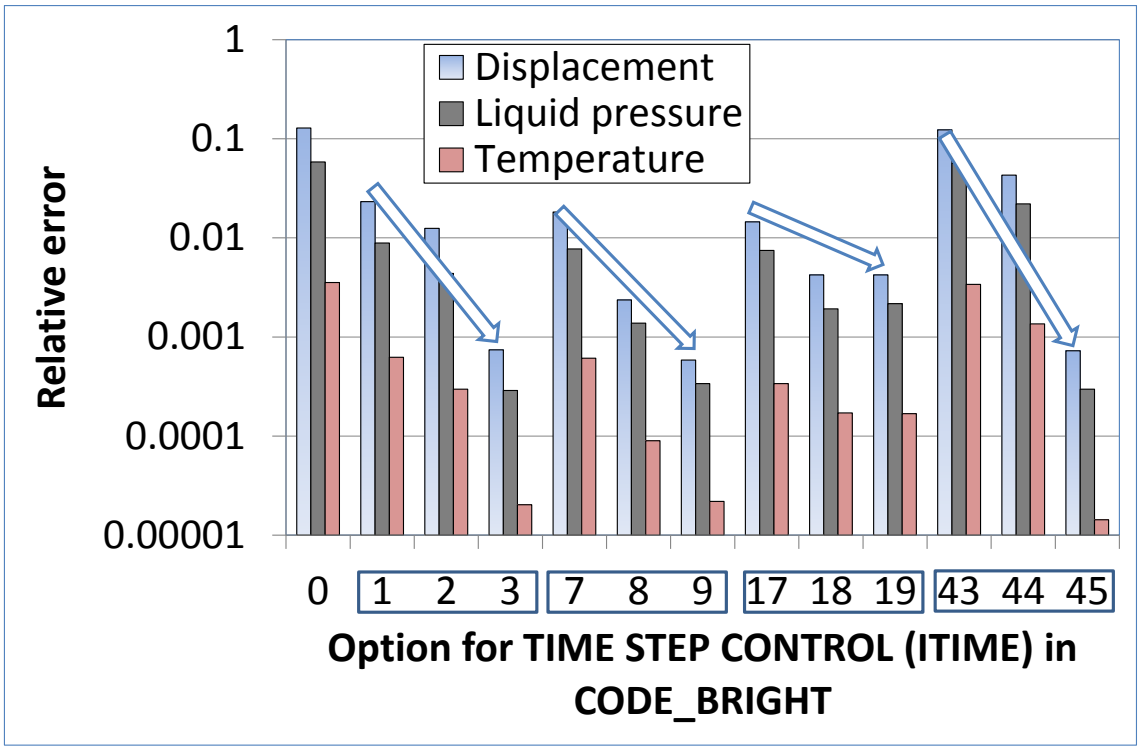
Evolution of time step during model run. The model uses (above) or not uses (below) the time step rejection method based large variations of calculated variables.

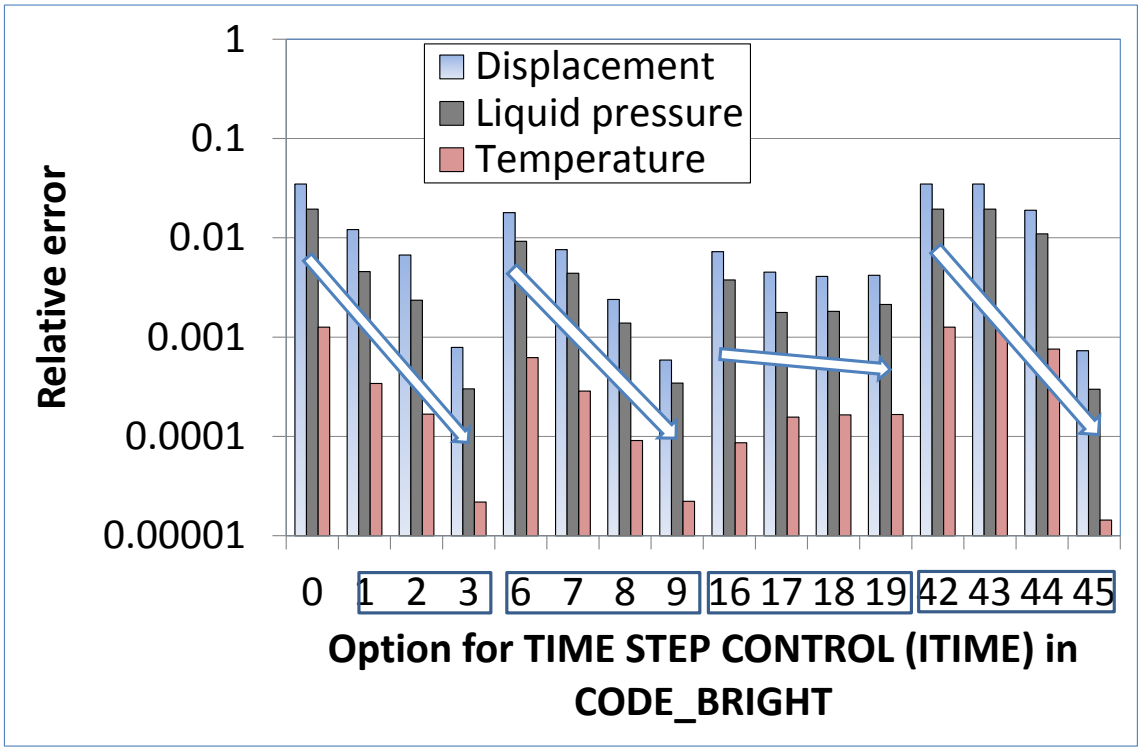


Time step rejections are 0 or very small when the variation of variables is not controlled. This implies less number of time steps (rejected time steps are counted because that implies CPU time consumption).



CPU time is smaller when variation control is not used. This increases de size of the time step (because the number or time steps is lower) and the number of NR iterations per time step.





Above: using time step rejections due to variation of variable limitted

Below: without time step rejections due to variation of variable limitted

The results indicate that time step variations are smoother when the time step rejections are minimized. In fact, some of the reductions which lead to a kind of catastrophic reduction (several concatenated time step reductions) still exist but are less catastrophic.

Total number of time steps is smaller when time step rejection is minimized, but the number of NR iterations per time step increases somewhat. However, globally, CPUTIME is smaller, i.e. the total number of NR iterations (product of average value by the number of time steps) is smaller.

Relative errors are compared and it is shown that minimizing rejections reduces the error. For instance, for option 7, relative errors are smaller that 10-3 for all variables when time step rejection was minimized and this was not the case in the preceding option.

Finally, rejection is not convenient because it increases CPUTIME and increases the RELATIVE ERROR of the solution.

7 Concluding remarks

Roughly all variables show similar response with respect to errors. Options 3, 9 and 45 give the best results for all plotted variables in terms of errors but at the same time produce a large CPU time consumption, between 5 and 9 times larger than the reference case 0. CPU time can be reduced if time step rejection is minimised.

Options 17, 18, 19 use second order approach for the time derivative of conservation equations. Results are not improving and the reason may be that the error is calculated with respect to a reference case which uses the first order approximation of the time derivative. This second order approximation has to be reviewed, probably by setting a different reference for the calculation of errors as we are obtaining a solution based on a different conservation equation in its numerical form.

Options 43, 44, 45, use error in stress calculation from integration subroutine of the constitutive model. The error is taken as equal to the last correction of stress obtained. This error estimate can be improved.

As a general conclusion it can be said that series 1 to 3 and 7 to 9 can be used for time step prediction. Series 17, 18, 19 and 43, 44, 45 require further refinements.

Among the options analysed, 2 and 8 are recommended. The average of NR iterations is 2.5 and 2, respectively. CPU time is acceptable for option 2 and can be considered in an affordable range for option 8. Option 18 gives similar results as 8, so it does not seem to improve. Options 43 or 44 can perhaps be interesting when the mechanical model is complex.

If time step control is adequate i.e. sufficiently restrictive, some of the time step rejection criteria are not necessary (will never go into a large number of NR iterations or will never get large variations of unknowns). By eliminating or minimizing time step rejections, calculation time is reduced and accuracy is improved.