Some notes on bgaPEST 09/12/2011

1. I think there is an error in Lines 30-32 of MAIN file.

```
if (cv_A%deriv_mode .eq. 1) then
  call bxd_write_ext_PEST_files(d_MOD, cv_MIO, d_MIO, cv_OBS, cv_PAR, d_OBS)
end if
```

According to documentation deriv_mode = 0 means use PEST, so if I understood well what `bxd_write_ext_PEST_files` does, in the IF statement we need `(cv_A%deriv_mode .eq. 0).` I didn't change this because you did and I'm not sure.

2. There are some issues related to the theta covariance stuff. See the file *theta_cov.pdf* uploaded to assembla for these problems.

3. For the structural parameter optimization loop, the convergence criterion that I implemented is now based on the norm of the differences between actual and previous theta vectors.

   ```
   curr_structural_conv(1)=sqrt(sum((curr_struct_vec - d_S%struct_par_opt_vec)**2))
   ```

   When this value is below `structural_conv` we exit the loop. Can this work or we have to monitore somethingh different?

4. I introduced a warning into the structural parameter subroutine if the minimum of the objective function (using Neal Meald) is not reached with the number of iterations entered by the user. The convergence of Neal-Meald routine is based on a value called REQMIN (that represent the terminating limit for the variance of function values) and it is set into the `marginal_struct_param_optim` subroutine (now is 10-2). We need to decide if leave this and the other Neal–Meald coefficients here or move them in a file.

The warning say: `'Warning: Maximum number of iterations exceeded in structural parameter optimization procedure during bgaPEST iteration',i4,'. The vector that gives the minimum obj. funct. during the procedure will be considered.'`

5. Now there is a control that in case we don't need structural parameter optimization and the number of iteration of the bga loop is greater than 1, returns a warning and ***it_max_bga*** is set to 1. What we should do if the structural parameter optimization is required and the user set ***it_max_bga*** to 1? Probably in this case ***it_max_bga*** should be at least 2 so the quasi-linear stuff run with the new structural parameters (after the first optimization I mean), even if they are not the best ones. What you think?

6. Look at the equation 26 of documentation I think there is an error. In the Lyx file you can found a note I wrote about this.

7. The subroutine that read sensitivity in case of ADJOINT, I think works fine just for the specific case we are using now (we should verify this). Probably we need to figure out a way (like an instruction file) to read sensitivity. We need also to have somewhere out of the code the name of the sensitivity file.

8. We need some warning if ***it_max_phi*** and ***it_max_bga*** are reached without convergence.