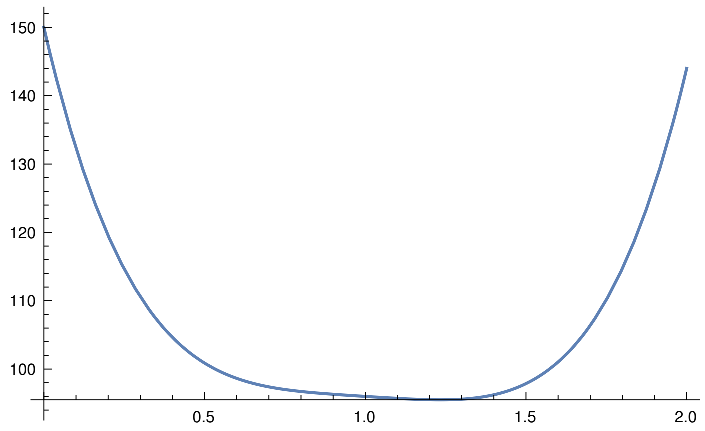
```
In[ ]:= (* Initialisation *)
(* Evaluate before starting writing "real code" *)
(* Usage e.g.: "ld [Spacekey]" becomes "⊨",
so writing "a ld 5" turns into "a⊨5" *)
SetOptions[EvaluationNotebook[],
            InputAutoReplacements → {(* special AceGen assignment operators: *)
   "ld" → "⊨", "ls" → "⊢", "rd" → "⫤", "rs" → "⊣",
                                    (* brackets and symbols: *) "dbl" → "〚",
   "dbr" → "〛", "lcb" → "{", "rcb" → "}", "lsb" → "[", "rsb" → "]", "->" → "→",
                                    (* shortcuts for
    starting/ending a comment block: *) "co" → "(*", "cc" → "*)"
                                   }
          ]
(* Output the current time,
so we know when AceGen has been executed the last time *)
Now

Out[ ]= Fri 14 Jun 2024 13:07:27 GMT+2

In[ ]:= (* Clear all old variables initially to have a fresh start *)
ClearAll["Global`*"]
(* Start AceGen *)
<< AceGen`;

NAME = "SMSDo_SMSD";
SMSInitialize[NAME, "Language" → "Matlab", "Mode" → "Optimal"];

(* Define the maximum number of Newton-Raphson iterations,
as this also defines the size of convergenceHistory$$ *)
n_iterations = 20;

(* Start a module, which represents the to be created function,
with name "NAME" and the specified input and output arguments *)
SMSModule[NAME, Real[displacement$$, parameter$$,
   convergedValue$$, convergenceHistory$$[2, n_iterations]],
          "Input" → {displacement$$, parameter$$},
          "Output" → {convergedValue$$, convergenceHistory$$}
         ];
displacement ⊨ SMSReal[displacement$$];
parameter ⊨ SMSReal[parameter$$];
```

In[∘]:=
```
(* Define some energy function and plot it with an exemplary parameter=1 *)
W_energy[utmp_, parameter_] := (1/2 * 100 * (utmp - parameter)^4 + utmp^2 - 5 utmp + 100);
Plot[W_energy[x, 1], {x, 0, 2}]
```

Out[∘]=



```
In[ ]:= (* #1 Works. *)
SMSDo[i_NR, 1, n_iterations, 1, displacement];
    (* Compute the energy to be minimised using the variable displacement *)
     W ⊨ W_energy[displacement, parameter];
    (* Find the mininum of the energy W by computing the slope of the
  energy which will be iteratively computed to find the minimum (R=0) *)
     R ⊨ SMSD[W, displacement];
    (* Give some output on the progress and export it to convergenceHistory$$ *)
     SMSPrintMessage["iteration i_NR=",
   i_NR, ": W=", W, "; R=", R, "; SMSAbs[R]=", SMSAbs[R]];
     SMSExport[displacement, convergenceHistory$$[i_NR, 1]];
     SMSExport[SMSAbs[R], convergenceHistory$$[i_NR, 2]];
    (* Check the residual for convergence *)
    SMSIf[ SMSAbs[R] < 1*^-8 ];
        SMSPrintMessage["converged"];
        (* Leave the SMSDo-Loop *)
        SMSBreak[];
    SMSEndIf[];
    (* If the maximum number of Newton-Raphson iterations is reached,
we output the current value and report a convergence failure *)
    SMSIf[ i_NR ≥ n_iterations];
        SMSPrintMessage["failed"];
        (* Leave the SMSDo-Loop *)
        SMSBreak[];
    SMSEndIf[];
    dRdu ⊨ SMSD[R, displacement];
    displacement ⊣ displacement - 1/dRdu * R;
SMSEndDo[displacement];

SMSExport[displacement, convergedValue$$];
SMSPrintMessage["du/dparameter_out =", SMSD[displacement, parameter]];
```

```
In[ ]:= (* #2 Wrong. The loop works, but the internal derivative is wrong.
   SMSDo[i_NR,1,n_iterations ,1,displacement];
     W ⊨ W_energy[displacement ,parameter];
     R ⊨ SMSD[W,displacement];
       (* Give some output on the progress and export it to convergenceHistory$$  *)
          SMSPrintMessage ["iteration  i_NR=",
  i_NR,": W=",W,"; R=",R, "; SMSAbs[R]=",SMSAbs[R]];
          SMSExport[displacement ,convergenceHistory$$ [i_NR,1]];
          SMSExport[SMSAbs[R],convergenceHistory$$ [i_NR,2]];
          (* Check the residual for convergence *)
     SMSIf[ SMSAbs[R]<1*^-8 ];
         SMSPrintMessage ["converged"];
         SMSExport[displacement ,convergedValue$$ ];
         SMSPrintMessage ["du/dparameter_in  =",SMSD[displacement , parameter]];
(* here the derivative is zero, because the downstream dependence
 of "displacement" on "R" and "R" on "parameter" is not seen *)
         SMSBreak[];
     SMSEndIf[];
           (* If the maximum number of Newton-Raphson iterations is reached,
we output the current value and report a convergence failure *)
           SMSIf[ i_NR ≥n_iterations];
         SMSPrintMessage ["failed"];
         SMSBreak[];
           SMSEndIf[];
     dRdu ⊨ SMSD[R, displacement];
     displacement ⊣ displacement - 1/dRdu * R;
SMSEndDo[];
*)
```

```
In[ ]:= (* #3 Wrong/zero subderivative inside, but correct derivative outside.
  SMSDo[i_NR,1,n_iterations,1,displacement];
    W ⊨ W_energy[displacement,parameter];
    R ⊨ SMSD[W,displacement];
      (* Give some output on the progress and export it to convergenceHistory$$ *)
         SMSPrintMessage["iteration i_NR=",
 i_NR,": W=",W,"; R=",R, "; SMSAbs[R]=",SMSAbs[R]];
         SMSExport[displacement,convergenceHistory$$[i_NR,1]];
         SMSExport[SMSAbs[R],convergenceHistory$$[i_NR,2]];
         (* Check the residual for convergence *)
    SMSIf[ SMSAbs[R]<1*^-8 ];
        SMSPrintMessage["converged"];
        SMSPrintMessage["du/dparameter_in =",SMSD[displacement, parameter]];
(* here the derivative is zero, because the downstream dependence
 of "displacement" on "R" and "R" on "parameter" is not seen *)
        SMSBreak[];
    SMSEndIf[];
          (* If the maximum number of Newton-Raphson iterations is reached,
we output the current value and report a convergence failure *)
          SMSIf[ i_NR ≥n_iterations];
        SMSPrintMessage["failed"];
        SMSBreak[];
          SMSEndIf[];
    dRdu ⊨ SMSD[R, displacement];
    displacement ⊣ displacement - 1/dRdu * R;
SMSEndDo[displacement];

SMSPrintMessage["du/dparameter_out =",SMSD[displacement, parameter]];
(* the outside derivative is correct *)
SMSExport[displacement,convergedValue$$];
*)
```

```
In[ ]:= (* #4 Works. Compute the local derivative
         using AD but with some manual help in two steps
         SMSDo[i_NR,1,n_iterations ,1,displacement ];
            W ⊨ W_energy[displacement ,parameter ];
            R ⊨ SMSD[W,displacement ];
            dRdu ⊨ SMSD[R, displacement ];
        (* Now compute dRdu directly here as it is needed in case of convergence *)
              (* Give some output on the progress and export it to convergenceHistory$$  *)
                 SMSPrintMessage ["iteration  i_NR=",
         i_NR,": W=",W,"; R=",R, "; SMSAbs[R]=",SMSAbs[R]];
                 SMSExport[displacement ,convergenceHistory$$ [i_NR,1]];
                 SMSExport[SMSAbs[R],convergenceHistory$$ [i_NR,2]];
                 (* Check the residual for convergence *)
            SMSIf[ SMSAbs[R]<1*^-8 ];
                SMSPrintMessage ["converged "];
                SMSPrintMessage ["dR/dparameter_in  =",
         SMSD[R, parameter , "Constant "→displacement ]];
        (* Computing dR/dparameter is possible as "R=R(parameter)" is known upstream. *)
                SMSPrintMessage ["du/dparameter_in  =",
         -1/dRdu * SMSD[R, parameter , "Constant "→displacement ]];
        (* Computing du/dparameter based on known update relation *)
                SMSBreak[];
            SMSEndIf[];
                  (* If the maximum number of Newton-Raphson iterations is reached,
        we output the current value and report a convergence failure *)
                  SMSIf[ i_NR ≥n_iterations ];
                SMSPrintMessage ["failed "];
                SMSBreak[];
                  SMSEndIf[];
            displacement ⊣ displacement - 1/dRdu * R;
        SMSEndDo[displacement ];

        SMSPrintMessage ["du/dparameter_out =",SMSD[displacement , parameter ]];
        SMSExport[displacement ,convergedValue$$ ];
        *)
```

```
In[ ]:= (* #5 Works. Change the order of the expressions. Note, several side effects!
  SMSDo[i_NR,1,n_iterations,1,displacement];
     W ⊨ W_energy[displacement,parameter];
     R ⊨ SMSD[W,displacement];
       (* Give some output on the progress and export it to convergenceHistory$$ *)
          SMSPrintMessage["iteration i_NR=",
  i_NR,": W=",W,"; R=",R, "; SMSAbs[R]=",SMSAbs[R]];
          SMSExport[displacement,convergenceHistory$$[i_NR,1]];
          SMSExport[SMSAbs[R],convergenceHistory$$[i_NR,2]];
     dRdu ⊨ SMSD[R, displacement];
          (* Now "displacement" is updated before checking for convergence *)
     displacement ⊣ displacement - 1/dRdu * R;
          (* Check the residual for convergence *)
     SMSIf[ SMSAbs[R]<1*^-8 ];
 (* Note that now the convergence check is done for R_k,
 which was computed from the old displacement (_k),
 not the updated one (_k+1) in the previous equation *)
         SMSPrintMessage["converged"];
         SMSPrintMessage["du/dparameter_in =",SMSD[displacement, parameter]];
 (* here the correct derivative is computed *)
         SMSBreak[];
     SMSEndIf[];
           (* If the maximum number of Newton-Raphson iterations is reached,
 we output the current value and report a convergence failure *)
           SMSIf[ i_NR ≥n_iterations];
         SMSPrintMessage["failed"];
         SMSBreak[];
           SMSEndIf[];
 SMSEndDo[displacement];

 SMSPrintMessage["du/dparameter_out =",SMSD[displacement, parameter]];
 SMSExport[displacement,convergedValue$$]; *)
```

```
In[ ]:= (* @todo Add more cases and explanations
  as there are many ways to do it wrong here *)
```

In[ ]:=
```
(* Output the time at the end of the execution *)
Now
(* Write output file containing all the
 above defined functions introduced by SMSModule *)
(* Create output file named "NAME", '"LocalAuxiliaryVariables " →
 True' is a command to exclude the AceGen internal array "v" from
  the list of input and output arguments of the created subroutine *)
SMSWrite[NAME, "LocalAuxiliaryVariables " → True];
(* Print the content of the just created
 file on screen (sensible only for small file sizes) *)
FilePrint[StringJoin[NAME, Which[SMSLanguage == "Fortran", ".f",
                                 SMSLanguage == "Matlab", ".m",
                                 SMSLanguage == "C++", ".cpp",
                                 SMSLanguage == "C", ".c"
                                ]
                     ]
          ]
```

Out[ ]= Fri 14 Jun 2024 13:07:31 GMT+2

File: SMSDo_SMSD .m **Size:** 1838 **Time:** 1

Method	SMSDo_SMSD
No.Formulae	17
No.Leafs	181

```
%**************************************************************
%* AceGen    7.505 Linux (16 Aug 22)                          *
%*           Co. J. Korelc  2020           14 Jun 24 13:07:31 *
%**************************************************************
% User     : Full professional version
% Notebook : AceGen-SMSDo_SMSD
% Evaluation time                 : 1 s     Mode   : Optimal
% Number of formulae              : 17      Method: Automatic
% Subroutine                      : SMSDo_SMSD size: 181
% Total size of Mathematica  code : 181 subexpressions
% Total size of Matlab code       : 940 bytes

%*********************** F U N C T I O N **************************
function[convergedValue,convergenceHistory]=SMSDo_SMSD(displacement,parameter);
persistent v;
if size(v)<148
  v=zeros(148,'double');
end;
v(20)=0;
v(1)=displacement;
for i3=1:1:20;
 v(5)=-parameter+v(1);
 v(23)=(v(5)*v(5));
 v(18)=2e0+600e0*v(23);
 v(6)=-5e0+2e0*v(1)+200e0*Power(v(5),3);
 disp(sprintf("\n%s  %f %s %f %s %f %s %f ","iteration  i_NR=",i3,":  W=",100e0-5e0*v(1)+(v(1)*v(
  +50e0*Power(v(5),4),";  R=",v(6),";  SMSAbs[R]=",abs(v(6))));
 convergenceHistory(i3,1)=v(1);
 convergenceHistory(i3,2)=abs(v(6));
 if(abs(v(6))<0.1e-7)
  disp(sprintf("\n%s  ","converged"));
  break;
 else;
 end;
 if(i3>=20)
  disp(sprintf("\n%s  ","failed"));
  break;
 else;
 end;
 v(20)=(1e0-2e0/v(18))*v(20)-(600e0*(-1e0+v(20))*(v(18)*v(23)-2e0*v(5)*v(6)))/Power(v(18),2);
 v(1)=v(1)-v(6)/v(18);
end;
convergedValue=v(1);
disp(sprintf("\n%s  %f ","du/dparameter_out=",v(20)));


function [x]=SMSKDelta(i,j)

if (i==j) , x=1; else x=0; end;

end

function [x]=SMSDeltaPart(a,i,j,k)

l=round(i/j);

if (mod(i,j) ~= 0 | l>k) , x=0; else x=a(l); end;

end

function [x]=Power(a,b)

x=a^b;

end

function [x]=SMSTernaryOperator(a,b,c)

if (c) , x=a; else x=b; end;

end

end
```