# THE EXTENDED VERSION OF CLASS COMBINEDSIMULATION

Below is given a brief description of the extended version of class `COMBINEDSIMULATION` (in the file XSIMULATION.sim).

The extensions are:

(1) the provision of a predictor-corrector integration method, namely Adams method with variable step-size and variable order.

(2) a virtual procedure, `PROLOGUE`, that is called automatically at the beginning of the simulation, and

(3) a variable, `DTSEV`, for specifying the time accuracy of state-events.

The extensions are indicated in the following class skeleton:

```
class COMBINEDSIMULATION;
virtual: procedure PROLOGUE;
begin
  procedure PROLOGUE;;
  Boolean ADAMS,RKE;
  integer MAXORDER;
  real DTSEV;
  .
  .
  ADAMS:=RKE:=false;
  MAXORDER:=12;
  DTSEV:=-1;
  PROLOGUE;
end;
```

### 1. Variable order Adams integration

A new integration method of the predictor-corrector type has been added to `COMBINEDSIMULATON`, namely Adams method with variable step size and variable order. The code is adapted from the excellent book by Shampine and Gordon (ref. 1) where a detailed description and analysis of the algorithms are provided together with well-documented FORTRAN code. This code is considered to be among the most efficient codes for the numerical solution of non-stiff differential equations. The actual implementation of Adams method in class `COMBINEDSIMULATION` is basically a SIMULA translation of this FORTRAN code. However, to fit the concepts of `COMBINEDSIMULATION`, some minor modifications have been made. These modifications mainly have to do with the integration error control and the reduction of round-off errors. The integration error is controlled as in the Runge-Kutta-England method; that is, in each VARIABLE-object, V, the local integration error must be less than

```
ABS(RELERROR*V.STATE)+ABS(ABSERROR)
```

(In contrast, the FORTRAN code uses the L2 norm). Round-off errors in `COMBINED-SIMULATION` are, as usual, reduced by using the quasi-double precision summation method.

Adams method is well-suited for solving non-stiff to mildly stiff differential equation systems. The method shows its true strength where evaluation of derivatives is expensive in terms of computer time, or where moderate to high accuracy is required. The method computes the derivatives only twice at each successful integration step, regardless of the order. (In comparison, the Runge-Kutta-England method makes 4.5 evaluations per step). The first evaluation is used for "prediction" using the Adams-Bashford method of order k. The second evaluation is used for "correction" using the Adams-Moulton method of order k+1.

The user selects Adams integration method merely by setting the Boolean variable `ADAMS` to `true`. Initially the value of `ADAMS` is `false`.

The local integration error will be controlled by varying the step size as well as the order of the Adams formula used. Typically changes of step size are limited to halving and doubling; changes of order, to one. The order varies between 1 and `MAXORDER`, where `MAXORDER` is an integer constant. The default value of `MAXORDER` is 12; however, if required, the value may be changed by the user.

The method is self-starting. At the start of the simulation and after a discrete event, the integration begins with the Adams formula of order one, requiring no memorized values. Usually the size of the first step is rather small, but typically the step size will double on successive steps until an appropriate step size is reached. However, if there are many discrete events in a simulation, this start procedure may be too inefficient. In such cases it may be better to use the Runge-Kutta-England integration method.To get the benefits of both integration methods, the Boolean variables RKE and ADAMS should be set to true. This causes the first step after every discrete event to be a Runge-Kutta-England step and the succeeding steps to be Adams steps. Initially `RKE` is false.

The fixed step size, second order Adams method is still available but must now be selected by setting the Boolean variable `FIXADAMS` to `true`. It should be noted that the variable order Adams method is selected only when `ADAMS` is `true` and `EULER`, `FIXADAMS`, `TRAPEZ` and `SIMPSON` are all `false`.

The Adams method uses a number of internal auxiliary variables. Thus each `VARIABLE`-object contains a real-valued array of size `MAXORDER+2`: `real array PHI(1:MAXORDER+2)`. In case the Adams method is not used and the storage requirement is important, the user may minimize storage consumption by setting `MAXORDER` to -1 at the very beginning of the simulation (or at least, before the `VARIABLE`-objects are generated). Maximum savings are obtained by setting `MAXORDER` to -1 in the procedure `PROLOGUE` (see below).

## 2. The virtual procedure PROLOGUE

PROLOGUE is a virtual procedure which is called automatically at the very start of the simulation. The procedure has been predefined with an empty procedure body.

## 3. Real DTSEV

The variable DTSEV may be used to specify the time accuracy of state-events. If DTSEV is not set by the user, or if it is given a negative value, then state-events will, as usual, be time-determined with an accuracy of DTMIN.

## Reference:

1 Shampine, L.F. and Gordon, M.K.:
"Computer solution of ordinary differential equations".
W.H. Freeman and Company, San Francisco, 1975.