Variable Step Variable Order Methods

- This material is adapted from J.D. Lambert, Numerical Methods for Ordinary Differential Systems, Wiley, 1991. That book and its references should be consulted for details.

- There are a number of ODE codes in the public domain. One of the oldest and best known is **lsode** (Livermore Solver of Ordinary Differential Equations, by Alan Hindmarsh). It consists of 3,390 lines of FORTRAN code and is a far cry from e.g., a simple Runge-Kutta code you might find in a simple-minded Numerical Analysis Text. There is a link to the code on our Canvas home page.

- A code of the same kind available in **matlab** is **ode113**

- **lsode** and related codes share the following ingredients:

  1. A family of methods
  2. A starting strategy
  3. A local error estimator
  4. A step-size/order policy
  5. A technique to change order
6. A technique to change step-size

- We discuss these items in turn.

1. **Family of Methods.**

- Choices of methods include
  - **Adams-Bashforth-Moulton Predictor Corrector Methods,** usually in
    
    $\begin{align*}
    PECE \quad \text{or} \quad P(EC)^2E
    \end{align*}$

    mode, with step-numbers ranging as high as 13, for **non-stiff** problems. In these notes, we will use the Adams methods to illustrate details of some of the other ingredients.

  - **Backward Differentiation formulas** of step-number up to 6 for **stiff problems,** combined with Newton’s method (and the accompanying linear algebra software) for solving the nonlinear systems.

  - **Blended Linear Multistep Methods,** a sophisticated combination of the two types above.

- The Adams Methods of order $k$ can be written as

  $$
  y_{n+1} = y_n + h \sum_{i=0}^{k-1} \gamma_i \nabla^i f_{n+1} \quad \text{(Adams-Moulton)}
  $$

  (1)
and
\[ y_{n+1} = y_n + h \sum_{i=0}^{k-1} \gamma_i^* \nabla^i f_n \]  
(Adams-Bashforth) \hfill (2)

where
\[ \nabla^0 f_n = f_n \quad \text{and} \quad \nabla^{i+1} f_n = \nabla^i f_n - \nabla^i f_{n-1} \]  
(3)

and the \( \gamma_i \) and \( \gamma^*_i \) are constants independent of the step-number \( k \).

2. A starting strategy.

- This is very simple, one starts with the one-step method. As the integration proceeds the step-number typically increases initially.

3. A local Error Estimator.

- Virtually all error estimation is based on the comparison of two approximations of the same quantity. The local error for initial value problems is
\[ E_{n+1} = y_{n+1} - z(x_{n+1}) \]  
(4)

where \( z \) is the exact solution of the differential equation that passes through the point \( (x_n, y_n) \). (The estimation of the global truncation error is much more difficult and not used in practice.) For predictor corrector methods this takes the form of Milne’s Device.
\[ y_{n+1} - y_n = h \sum_{j=0}^{k} \beta_j f_{n-k+1+j} \]
For the Adams Methods the error estimate is very simple:

\[ E_{n+1} = h \gamma_k \tilde{\nabla}^k f_{n+1} \]  

(5)

where \( \tilde{\nabla}^k f_{n+1} \) is just \( \nabla^k f_{n+1} \) with \( f_{n+1} \) replaced by \( f_{n+1}^{[0]} \), i.e., \( f \) evaluated at the predicted value. Note that this can be evaluated at the PEC stage of the PECE computation, so that the final evaluation can be omitted if the estimated error is too large.


- Suppose the last step was taken at step-number \( k \) and step-size \( h \). Depending on the particular code, the step is accepted if either

\[ \| E_{n+1} \| \leq \tau \]  

(6)

or

\[ \| E_{n+1} \| \leq \tau h. \]  

(7)

where \( \tau \) is a user specified quantity that governs the accuracy of the integration. For the sake of this illustration let us consider the requirement (6). The reasoning can be extended easily to the requirement (7). Whether the step is accepted or not the maximum allowable step-sizes \( h_{k+i}^* \), \( i \in \{-1, 0, 1\} \) are now estimated for the step number \( k + 1, k \), and \( k - 1 \). Whichever of these three maximum step-lengths turns out to be the largest will
determine the step-number and step-size at the next step. (The actual step taken will be a little less than the estimated maximum step-size, to reduce the risk of a marginal rejection.) Let \( E_{n+1}^{k+i}, i \in \{-1, 0, 1\} \) denote the estimated error for the three contemplated step-numbers. It turns out that the following computable asymptotic\(^{-1}\) estimates hold:

\[
E_{n+1}^{k+i} = h \gamma_{k+i} \tilde{\nabla}^{k+i} f_{n+1}.
\] (8)

By the definition of order, the maximum step-sizes satisfy

\[
\tau = K_{k+i} (h^*_{k+i})^{k+i+1}
\] (9)

for some constants \( K_{k+i} \). Similarly,

\[
\|E_{n+1}^{k+i}\| = K_{k+i} h^{k+i+1}.
\] (10)

We can solve these two equations for \( h^*_{k+i} \) to give

\[
h^*_{k+i} = h \left( \frac{\tau}{\|E_{n+1}^{k+i}\|} \right)^{k+1+i}. \quad \text{(11)}
\]

As already stated above, we now pick the order corresponding to the largest \( h^*_{k+i} \) and a slightly smaller step-size for the next step.

\(^{-1}\) Without going into too much detail, the term asymptotic in this context means that the approximation becomes exact in the limit as the step-size \( h \) tends to zero.
5. A technique to change order.

- A change of order is implemented very simply by adding or omitting a term in (1) and (2).

6. Two techniques to change step-size.

- For a long time the stumbling block in developing linear multistep methods were the difficulties in changing the step-size. Two techniques evolved as viable:
  
  a. **Interpolation** (in $f$) to generate missing back values.
  
  b. Computation of the coefficients of a **new Adams-type method** specifically for the current combination of unevenly spaced back values.