Gear's Method for Integrating Stiff Systems

The stability region of an A-stable method includes the negative hc-half-plane. Demanding A-stability restricts the global error order of methods suitable for integrating stiff systems. For this reason, several modified stability notions have been introduced which are related to A-stability, but allow to increase the global error order of a method.

Gear's method is based on the characteristic polynomial

(1) $P(\lambda) = \rho(\lambda) - hc\sigma(\lambda)$

At first σ(x) is chosen in such a way that P(λ) -> 0 as Ihcl -> ∞ : Division of (1) by hc and taking the limit Ihcl -> ∞leads to σ(λ) = 0. The simplest choice is

(2) $\sigma(\lambda) = \lambda^M$

For this reason, P(λ) has the best possible stability property for hc = ∞: If Ihcl = ∞, P has an M-fold root at λ = 0. The condition of strong absolute stability (see fig. 3) is fulfilled at hc = ∞. In order to determine the behavior at finite points of the hc-plane, one has to

1) find the polynomial P(λ) and thus ρ(λ), and
2) to determine its stability region.

> **DEFINITION 17.18** (*Absolute stability, stability for h ≠ 0*).
> An algorithm for the numerical integration of (17.1) is *strongly absolutely stable* for a fixed $h \neq 0$, if all roots λ_ν of (17.27) satisfy $|\lambda_\nu| < 1$. It is called *weakly absolutely stable*, if the root condition of Definition 17.17 is fulfilled, otherwise it is *unstable*.
> A curve in $\mathbb{R}^2$ which bounds the region of absolute stability of a method is called its *stability boundary*, see also [ENGE87], p. 458.

Fig. 3

1) For (2) one can calculate the associated ρ(x) from the consistency conditions : A linear multi-step method has the consistency order q, if (see fig.4):

$$(17.33) \quad \begin{cases} (i) \quad \sum_{k=0}^{M} \left(a_k k^j - j b_k k^{j-1} \right) = 0, \ j = 1, \ldots, q, \ \text{and} \\ (ii) \quad \sum_{k=0}^{M} a_k = 0. \end{cases}$$

Fig. 4

(17.33) is a system of q+1 linear equations for the coefficients ak, k = 0,...,q, of the multi-step procedure.

2) The stability region of the multi-step method obtained by solving the linear system in 1) is determined for $\lambda = re^{i\phi}$ with $|\lambda| = r \leq 1$ from (see fig.5)

$$
(17.33) \quad
\begin{cases}
(i) & \sum_{k=0}^{M} \left(a_k k^j - jb_k k^{j-1}\right) = 0, \; j = 1, \ldots, q, \text{ and} \\
(ii) & \sum_{k=0}^{M} a_k = 0.
\end{cases}
$$

Fig. 5

The stability boundary is obtained by setting r = 1.

Corrector formulas of Gear's method for q = 1,...,6.

The iteration rules for the various methods are given below (see fig. 6) for $\sigma(\lambda) = \lambda^M$,

M = 1,...,6, with M = q as consistency order :

M	Corrector formulas of Gear's method for $q = 1, \ldots, 6$	
1	$Y_{i+1}^{(\nu+1)} = Y_i + hf_{i+1}^{(\nu)} = Y_i + hf(x_{i+1}, Y_{i+1}^{(\nu)}),$	$\nu = 0, 1, 2, \ldots$
2	$Y_{i+1}^{(\nu+1)} = \frac{1}{3}\left(4Y_i - Y_{i-1} + 2hf_{i+1}^{(\nu)}\right),$	$\nu = 0, 1, 2, \ldots$
3	$Y_{i+1}^{(\nu+1)} = \frac{1}{11}\left(18Y_i - 9Y_{i-1} + 2Y_{i-2} + 6hf_{i+1}^{(\nu)}\right),$	$\nu = 0, 1, 2, \ldots$
4	$Y_{i+1}^{(\nu+1)} = \frac{1}{25}\left(48Y_i - 36Y_{i-1} + 16Y_{i-2} + \right.$ $\left. -3Y_{i-3} + 12hf_{i+1}^{(\nu)}\right),$	$\nu = 0, 1, 2, \ldots$
5	$Y_{i+1}^{(\nu+1)} = \frac{1}{137}\left(300Y_i - 300Y_{i-1} + 200Y_{i-2} + \right.$ $\left. -75Y_{i-3} + 12Y_{i-4} + 60hf_{i+1}^{(\nu)}\right),$	$\nu = 0, 1, 2, \ldots$
6	$Y_{i+1}^{(\nu+1)} = \frac{1}{147}\left(360Y_i - 450Y_{i-1} + 600Y_{i-2} + \right.$ $\left. -225Y_{i-3} + 72Y_{i-4} - 10Y_{i-5} + 60hf_{i+1}^{(\nu)}\right),$	$\nu = 0, 1, 2, \ldots$

Fig. 6

For q = 1,...,6 only one functional evaluation of f is necessary per iteration step. The stability regions for q = 1,...,6 are given in the following picture (see fig. 7). Every boundary curve of a stability region passes through the points as Ihcl = ∞ of the hc-plane as shown in figures 7 and 8. For M = 2 the method is weakly A-stable, as in Heun's method. The formulas are stiffly stable for M = 3,...,6.
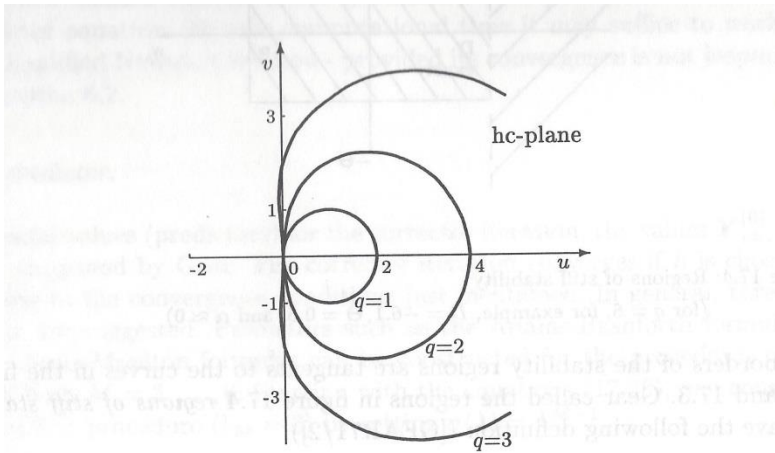
Fig. 7

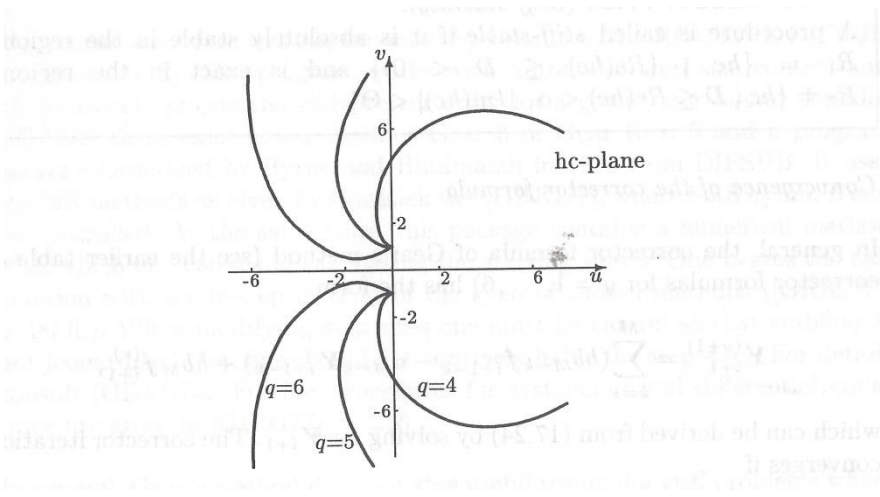Fig. 8

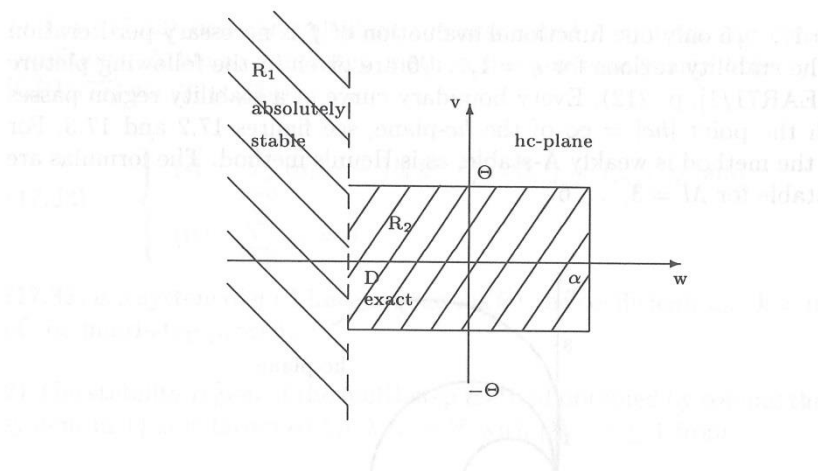One can represent the stability regions for the methods of Gear in a simplified way as follows:

Fig. 9 Regions of stiff stability (for q=6, for example, D =-6.1, θ = 0.5 and α ~ 0)

The borders of the stability regions are tangents to the curves in the figures 7 and 8. Gear called the regions in figure 9 regions of stiff stability. He gave the following definition:

DEFINITION 17.21 (*Stiff stability*).
A procedure is called *stiff-stable* if it is absolutely stable in the region $R_1 = \{hc \mid (Re(hc) \leq D < 0)\}$ and is exact in the region $R_2 = \{hc \mid D \leq Re(hc) < \alpha, |Im(hc)| < \Theta\}$.

Convergence of the corrector formula

In general, the corrector formula of Gear's method has the form

$$Y_{i+1}^{(\nu+1)} = \sum_{k=1}^{M}(hb_{M-k}f_{i+1-k} - a_{M-k}Y_{i+1-k}) + hb_M f_{i+1}^{(\nu)},$$

which can be derived from (17.24) by solving for Y_{i+1}. The corrector iteration converges if

$$\left\|hb_M\left(\frac{\partial f_i}{\partial y_k}\right)\right\| < 1,$$

where $\left(\frac{\partial f_i}{\partial y_k}\right)$ is the Jacobi matrix and $\|\cdot\|$ a matrix norm. For stiff single differential equations, as well as for separated differential equations, the convergence condition becomes

$$h\left|b_M\frac{\partial f}{\partial y}\right| < 1.$$

The convergence condition for the iteration might demand a smaller h than is resuired by the stiffly-stable method used. In this case, one should use Newton's method instead of the general iteration procedure for solving the corrector equation. To save computational time it may suffice to work with the simplified Newton's method – provided its convergence is not jeopardized.

The predictor   *(0)*

As initial values (predictors) for the corrector iteration, the values Y i+1 = Y I were suggested by Gear. The corrector iteration converges if h is chosen according to the convergence conditions just mentioned. In general, three iterations are suggested. Predictors such as the Adams-Bashforth formulas for the Adams-Moulton formulas can be constructed for the procedures of Mth order with M = 3,…,6: Starting with the equations (17.33), see fig. 5, one constructs an explicit procedure (bM = 0) by setting σ(λ) = λ M-1.

Remarks for Gear's method

The whole procedure was implemented by Gear. The program works with automatic step size control and automatically selects the global error order for a given error bound.

In general, Gear's method does not give useful results for stiff problems where the eigenvalues λ I of the Jacobi matrix (f y) are close to the imaginary axis of the hc-plane. For then some eigenvalues are outside of or close to the boundary of the region of absolute stability. In this case, Rosenbrock's methods have proven useful.

From [BIBLI 11].