Numerical Schemes for Time Integrations -- Solving Initial Value Problems

Explicit Scheme:

- The future information are determined based on the present and the past information
- Easy to program, easy to blowout!
- To avoid blowout, one have to choose shorter time step.
- A short time step means more CPU time

Implicit Scheme:

- The future information are determined based on the future, the present, and the past information
- Difficult to program and/or require more memory
- Stable in large time step.
- Implicit scheme can save more CPU time and provide reliable results

Predictor-Corrector Method Based on Adams Formula

Predictor-Corrector method is an easy-to-program implicit scheme, but require more memory than the corresponding explicit scheme. We use the Adams' formula to construct the Predictor-Corrector simulation scheme

The 4^{th} order Predictor-Corrector method recommended by Shampine and Gordon, (1975) is summarized below.

Procedure of the 4th order Predictor-Corrector Method

Initial	Solving $dy/dt = f$ or $\partial y/\partial t = f$ with $h = \Delta t$ to obtain y^1, y^2, and y^3 from y^0 by the 4th order Runge-Kutta method
Predicting Step	Predicting y^{n+1} from y^n, y^{n-1}, y^{n-2}, and y^{n-3} by the 4th order Adams Open Formula: $y^{n+1} = y^n + h[\frac{55}{24} f^n - \frac{59}{24} f^{n-1} + \frac{37}{24} f^{n-2} - \frac{9}{24} f^{n-3}] + O(h^5 f^{(4)})$
Correcting Steps	Correcting y^{n+1} from y^{n-2}, y^{n-1}, y^n, and the last y^{n+1} by the 4th order Adams Close Formula: $y^{n+1} = y^n + h[\frac{9}{24} f^{n+1} + \frac{19}{24} f^n - \frac{5}{24} f^{n-1} + \frac{1}{24} f^{n-2}] + O(h^5 f^{(4)})$
	Repeat the *Correcting* step until *the iteration converges*.
...	Repeat the *Predicting* and *Correcting Steps* to advance y from y^n to y^{n+1}.

The 4th order Runge-Kutta method (an explicit scheme)

Solving $dy/dt = f$ or $\partial y/\partial t = f$ with $h = \Delta t$

$$(y^*)^{n+\frac{1}{2}} = y^n + \frac{h}{2} f(t^n, y^n)$$

$$(y^{**})^{n+\frac{1}{2}} = y^n + \frac{h}{2} f(t^{n+\frac{1}{2}}, (y^*)^{n+\frac{1}{2}})$$

$$(y^{***})^{n+1} = y^n + h f(t^{n+\frac{1}{2}}, (y^{**})^{n+\frac{1}{2}})$$

$$y^{n+1} = y^n + h[\frac{1}{6} f(t^n, y^n) + \frac{2}{6} f(t^{n+\frac{1}{2}}, (y^*)^{n+\frac{1}{2}})$$
$$+ \frac{2}{6} f(t^{n+\frac{1}{2}}, (y^{**})^{n+\frac{1}{2}}) + \frac{1}{6} f(t^{n+1}, (y^{***})^{n+1})] + O(h^5 f^{(4)})$$

References

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Press, W. H., B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes (in C or in FORTRAN and Pascal), Cambridg*e University Press, Cambridge, 1988.

Shampine, L. F., and M. K. Gordon, *Computer Solution of Ordinary Differential Equation: the Initial Value Problem,* W. H. Freeman and Company, San Francisco, 1975.