Aleksandar Jemcov

Application of Vector Sequence Extrapolation to Iterative Algorithms in Computational Fluid Dynamics

10 Cavendish Court
Lebanon
NH
03766
USA
aj@fluent.com
Joseph P. Maruszewski

The vector extrapolation methods are the generalization of the Aitken's $\triangle^2$ method for the scalar equations that allow a significant acceleration of the monotonic convergence. The idea of the convergence acceleration through the extrapolation methods is based on the transformation of a slowly converging sequence $\{X_i\}$ into a new sequence $\{Y_i\}$ converging to the same limit faster than the initial one. The transformation

$$T : \{X_i\} \rightarrow \{Y_i\} \tag{1}$$

is constructed by interpolating a finite number of terms in the sequence $\{X_i\}$, thus effectively computing the sequence limit through the following linear combination:

$$s = \sum_{i=0}^{k} \alpha_i X_i. \tag{2}$$

The vector extrapolation methods extend this approach to the sequences whose elements are vectors in the same way they were used in Eq. (2) to accelerate the scalar sequences. Weighting coefficients α_i are determined by minimizing the error terms defined as the difference between the limit of the sequence s and the arbitrary elements of the sequence X_i:

$$\epsilon_i = s - X_i. \tag{3}$$

For the linear fixed-point functions this is achieved by observing that the initial error ϵ_0 can be related to the subsequent error ϵ_i through the powers of the iteration matrix of the fixed-point function:

$$\epsilon_i = \mathcal{R}^i \epsilon_0. \tag{4}$$

Here the fixed point function is defined by

$$X_{i+1} = \mathcal{R} X_i + b. \tag{5}$$

If we take the definition of the error, Eq. (3) and observing that the arbitrary element of the sequence can be expressed as

$$X_i = s - \mathcal{R}^i \epsilon_0, \tag{6}$$

and if we substitute Eq. (5), we can arrive to the conditions that the weighting coefficients must satisfy in order to minimize the error in Eq. (2):

$$\sum_{i=0}^{k} \alpha_i X_i = s \sum_{i=0}^{k} \alpha_i - \sum_{i=0}^{k} \alpha_i \mathcal{R}^i \epsilon_0. \tag{7}$$

Eq. (7) is equivalent to the following constrained minimization problem:

$$\alpha = argmin(\alpha_i) || X_0 + \sum_{i=0}^{k} \alpha_i \triangle X_i || \tag{8}$$

such that

$$\sum_{i=0}^{k} \alpha_i = 1. \tag{9}$$

In other words, Eq. (7) corresponds to finding the coefficients of the minimal polynomial associated with the iteration matrix $\mathcal{R}$ and this indicates an intimate link between vector sequence extrapolation and Krylov subspace methods. Another point of view that we will be taking here is that the vector sequence extrapolation methods correspond to the preconditioned Krylov subspace methods that use the fixed-point algorithms as the nonlinear preconditioners.

Strictly speaking, Eq. (5) is valid for the linear fixed point functions but the method can be extended to the nonlinear fixed point functions through a local linearization and by the inclusion of restarts in the algorithm. The general form of the nonlinear fixed-point functions considered here takes the following form:

$$X_{i+1} = \mathbf{F}(X_i). \tag{10}$$

Using the local linearization, the initial and i-th error are related through the powers of the Jacobian of the fixed point function with the second order accuracy, similarly to Eq. (4):

$$\epsilon_i = \partial_X \mathbf{F}^i (X_i) \epsilon_0 \tag{11}$$

The nonlinearly preconditioned Krylov subspace method algorithm can be devised that is similar to the algorithm described in Eq. (8) and Eq. (9) but with the use of restarts.

The vector extrapolation method is applied to problems in Computational Fluid Dynamics and it is shown that it leads to a significant acceleration of the convergence rates. Moreover, the method can be applied to the acceleration of any fixed-point algorithm with the minimal or no changes to the original algorithm. Results are demonstrated for the cases of the compressible and incompressible flows as well in conjunction with the explicit and implicit algorithms.