Chapter 1

Jacobian-Free Newton-Krylov Solver

A Jacobian-Free Newton-Krylov (JFNK) solver is a generic name for an algorithm that solves a system of nonlinear equations. As implied by the name, these solvers are defined by two main characteristics: lack of a need to form the exact Jacobian and Newton-like updates obtained from a Krylov method. Since the ability to avoid creating the exact Jacobian comes directly from using a Krylov method, a brief overview of those methods will be given before discussing the particular method leveraged in this work's JFNK solver: Generalized Minimal Residual (GMRES).

1.1 Krylov Methods

Krylov methods are a class of techniques used to solve linear systems of the form

$$Ax = b \tag{1.1}$$

where x and b are $N \times 1$ vectors and A is an $N \times N$ nonsingular matrix. Different methods place other limitations on A, but the most general condition (and the only condition required by GMRES) is that the coefficient matrix be invertible. The exact solution to equation 1.1 is, trivially,

$$x = A^{-1}b. \tag{1.2}$$

However, if N is large, the exact inversion of A can be computationally and memory intensive. The computational cost of inverting A is only exacerbated when solving nonlinear problems with a Newton-like scheme since several, if not many, linear solves are required to make one nonlinear advancement in the solution.

The solution in equation 1.2 will now be rewritten in a form that expresses the solution as a correction from some arbitrary initial guess and is inverse-free. Given an initial guess vector x_0 with an associated residual vector $r_0 = b - Ax_0$, a new vector $\tilde{x}$ can be created by shifting in a direction Δx off of the guess vector: $\tilde{x} = x_0 + \Delta x$. If the new vector is not the solution to the problem, the shift induces a new residual $\tilde{r}$ of the form

$$\tilde{r} = r_0 - A\Delta x. \tag{1.3}$$

If $\tilde{x}$ is the true solution x, the induced residual $\tilde{r}$ is precisely 0, and the shift is therefore $\Delta x = A^{-1}r_0$. The solution can then be written in a guess-correction form (where the correction is such that the induced residual is 0):

$$x = x_0 + A^{-1}r_0. \tag{1.4}$$

This form of the solution still presents the problem of forming A's inverse. To avoid this problem, we use a result of the Cayley-Hamilton theorem: the inverse of a square, $N \times N$ matrix can be expressed as a linear combination of the matrix's powers from 0 to $N-1$. To wit, the inverse of matrix A satisfies the equality

$$A^{-1} = \sum_{i=0}^{N-1} c_i A^i \tag{1.5}$$

assuming the weights c_i are chosen properly. Substituting this expansion into equation 1.4 yields

$$\tilde{x} = x_0 + \sum_{i=0}^{N-1} c_i A^i r_0. \tag{1.6}$$

The set vectors $\{r_0, Ar_0, A^2r_0, \cdots, A^{N-1}r_0\}$ is called the Krylov Subspace and will be denoted by $\mathcal{K}_N(A, r_0)$

1.2 GMRES

1.2.1 Algorithm

1.3 Jacobian-Free Augmentation