What this code is about

The Padé approximant to a given formal power series expansion $\sum_{n=0}^{\infty} a_n\beta^n$, is given by

$$P_M^N(\beta) = \frac{\sum_{n=0}^{N} A_n\beta^n}{\sum_{n=0}^{M} B_n\beta^n}, \quad B_0 = 1, \tag{1}$$

where

$$\mathbf{M}\begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_M \end{bmatrix} = -\begin{bmatrix} a_{N+1} \\ a_{N+2} \\ \vdots \\ a_{N+M} \end{bmatrix}, \tag{2}$$

With $\mathbf{M}_{i,j} = a_{N+i-j}(1 \le i, j \le M)$. The coefficients in the numerator are

$$A_n = \sum_{j=0}^{n} a_{n-j}B_j, \quad 0 \le n \le N. \tag{3}$$

The C++ code pade.cpp computes the Padé approximant (1) for $\beta = 10^{-5} - 10^{23}, 0.2$ and $\beta = 4$. The coefficients B_j are read in from the file Constant.txt while the coefficients a_j are read in from the file moments.txt. The result for $P_M^N(\beta)$ are written to pade.txt. We apply the Pade approximant to the energy correction of the ground-state energy of the quartic anharmonic oscillator,

$$E^{(2)}(\beta) = 1 + \sum_{k=1}^{\infty} b^{(k)}\beta^k = 1 + \beta\sum_{k=0}^{\infty} b^{(k+1)}\beta^k. \tag{4}$$

The file compile.job is a SLURM script to compile the code in an HPC and generate an executable.

The file together.job is a SLURM script to run the executable in an HPC.