What this code is about

The C++ code moments.cpp computes the Rayleigh-Schrodinger perturbation expansion coefficients b_k

$$E(\beta) = 1 + \sum_{k=1}^{\infty} b_k \beta^k \tag{1}$$

for the ground-state energy of the sextic anharmonic oscillator. We computed up to $k = d, d-1, ..., 1$ recursively using the following formulae,

$$b_0 = 1, \qquad b_1 = \frac{15}{8} \tag{2}$$

$$b_k = \frac{54\sqrt{2}}{8} a_{0,2}^{(k-1)} + \frac{15\sqrt{4!}}{8} a_{0,4}^{(k-1)} + \frac{\sqrt{6!}}{8} a_{0,6}^{(k-1)}, \qquad k \geq 2. \tag{3}$$

Where

$$a_{0,m}^{(0)} = 0, \qquad a_{0,m}^{(1)} = -\frac{\langle m|x^6|0\rangle}{2m} \tag{4}$$

$$a_{0,m}^{(r)} = -\frac{1}{2m}\left(\sum_{k=1}^{\infty} \langle m|x^6|k\rangle\, a_{0,k}^{(r-1)} - \sum_{s=1}^{r-1} a_{0,m}^{(s)}\, b_{r-s}\right), r \geq 2,\ m \neq 0,$$

the infinite sum becomes finite since the following are the only non-zero matrix elements,

$$\langle n|x^6|n+6\rangle = \frac{1}{8}\sqrt{(n+6)(n+5)(n+4)(n+3)(n+2)(n+1)} \tag{5}$$

$$\langle n|x^6|n+4\rangle = \frac{3}{8}\sqrt{(n+4)(n+3)(n+2)(n+1)}(2n+5) \tag{6}$$

$$\langle n|x^6|n+2\rangle = \frac{15}{8}(n^2+3n+3)\sqrt{(n+1)(n+2)} \tag{7}$$

$$\langle n|x^6|n\rangle = \frac{5}{8}\left(4n^3+6n^2+8^n+3\right) \tag{8}$$

$$\langle n|x^6|n-2\rangle = \frac{15}{8}\sqrt{n(n-1)}(n^2-n+1) \tag{9}$$

$$\langle n|x^6|n-4\rangle = \frac{3}{8}\sqrt{n(n-1)(n-2)(n-3)}(2n-3) \tag{10}$$

$$\langle n|x^6|n-6\rangle = \frac{1}{8}\sqrt{n(n-1)(n-2)(n-3)(n-4)(n-5)} \tag{11}$$

The coefficients b_k are written to the file moments.txt.

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.

The file mpfr.sh is a shell script used to compile and run the code in an Ubuntu 22.04 local machine.