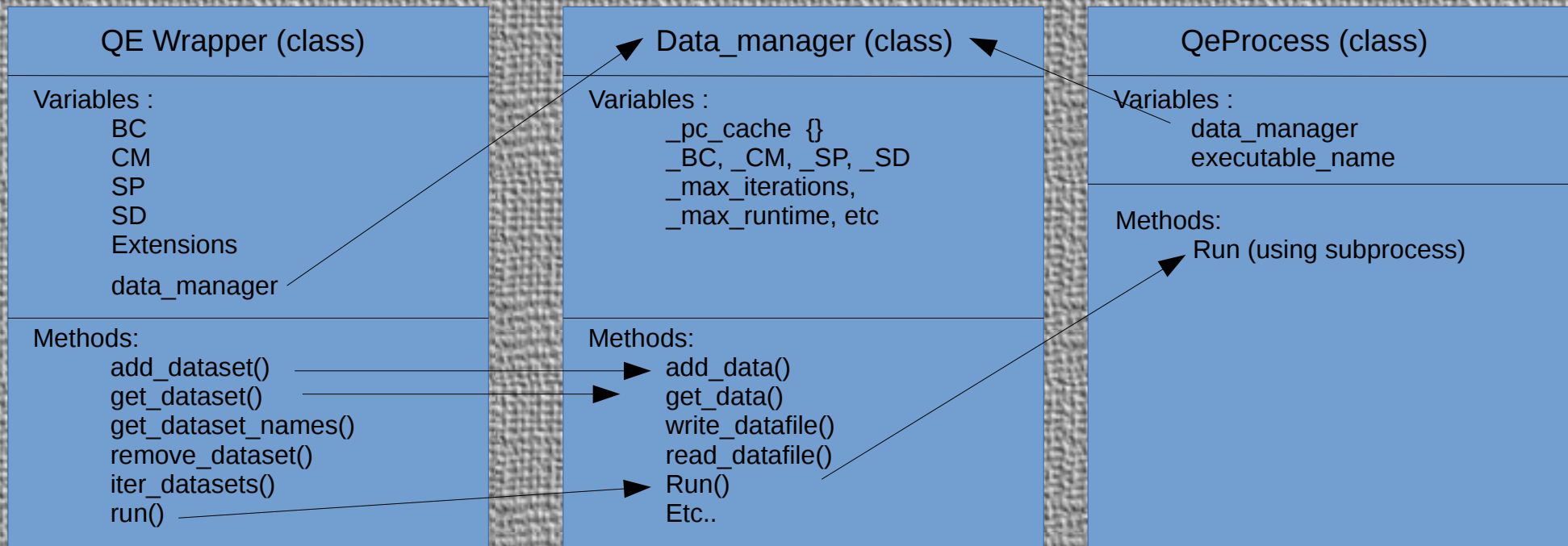


Indulgence by Proxy



```
Mywrapper= QeWrapper()
pc=Particles('buckyball')
p = Particle(coordinates=[0,1,2])
pc.add_particles(p)
Mywrapper.add_dataset(pc)
Mywrapper.run() ...
```

data_in.qe

QUANTUM
ESPRESSO

data_out.qe

```
...Mywrapper.run()
Data = Mywrapper.get_dataset('buckyball')
tot_energy = data['energy']
```