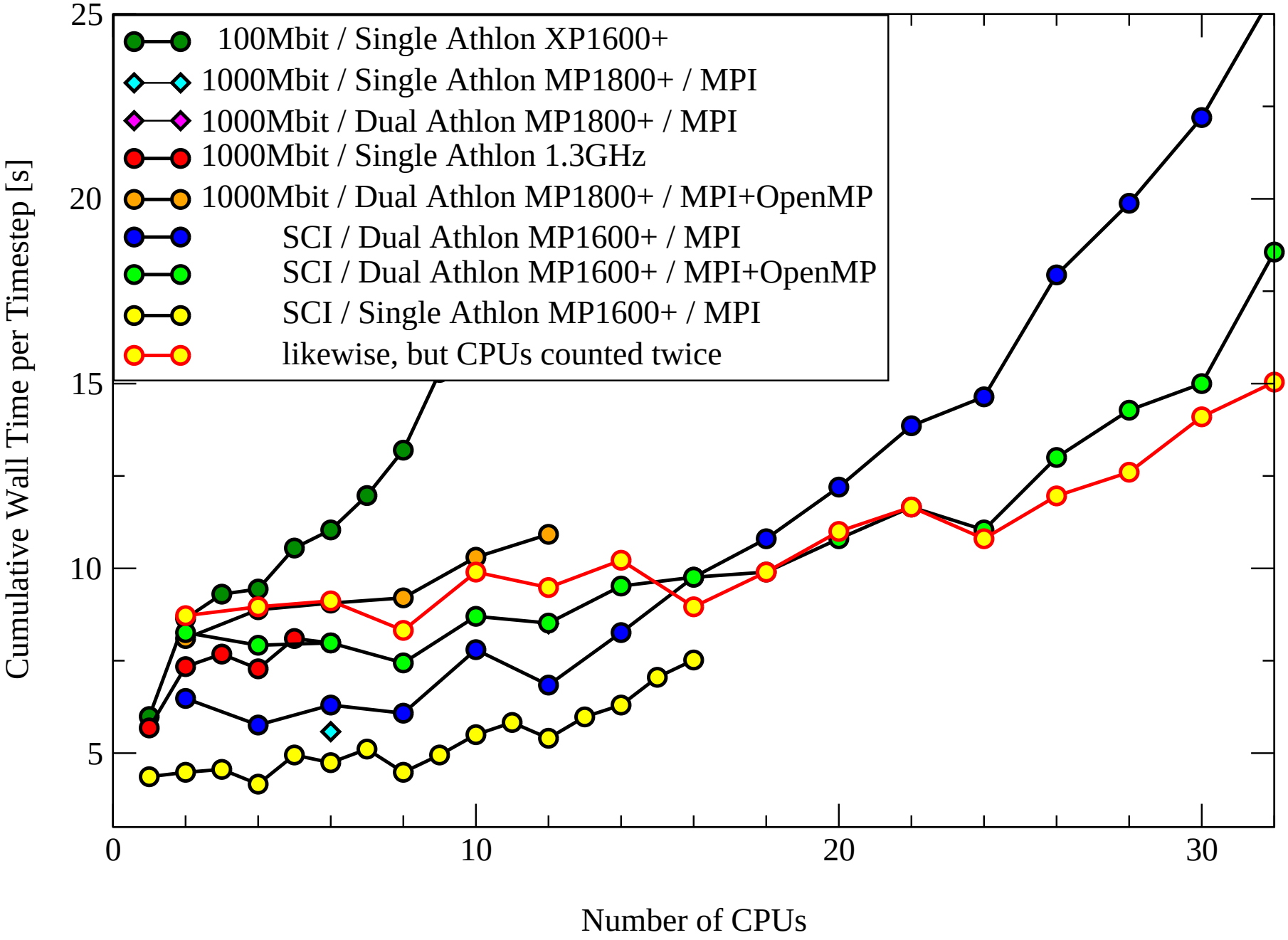Si_63 bulk / PBC / 10 Ryd