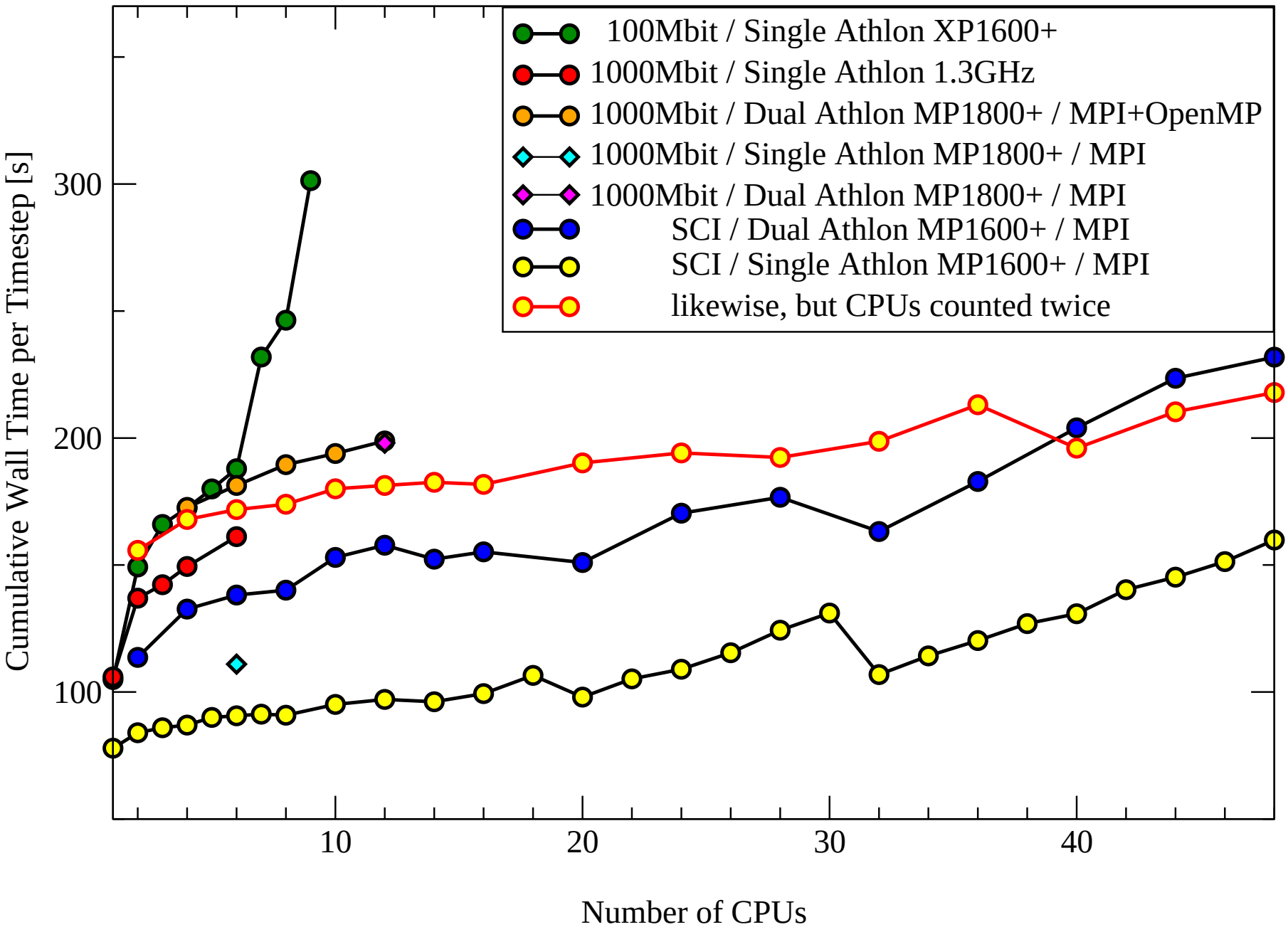Si_63 bulk / PBC / 70 Ryd