For the dynamics without RTA.

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|---|---|
| energies.<name> | historical, contains only the binding energy |
| forces.<name> | forces on ions, generated when ion molecular dynamics is active |
| <name>.bs | not found |
| pdip.<name> | dipole moment in x, y, z direction, versus time |
| penerclu.<name> | kinetic energy of the cluster in the x,y,z directions and total, versus time, at intervals commanded by the input parameter jener |
| pescel.<name> | proportion of electrons remaining, total number of electrons, number of electrons lost, versus time, at intervals commanded by the input parameter jesc |
| plaser.<name> | laser parameters Ex, Ey, Ez, power, laser energy, etc as a fonction of time |
| povlp.<name> | unused in this version |
| penergies.<name> | Various energies, versus time. The 26 detailed entries (single particle energy, rearrangement energy, etc..) are described in the output file itself. The total energy is at location 18. |
| pescOrb.<name> | Number of electrons lost per orbital, versus time, at intervals commanded by the input parameter jnorms |
| pkinenion.<name> | kinetic energy of the cluster in the x,y,z directions and total, versus time, at intervals commanded by the input parameter jpos |
| pPES.<name> | unused in this version |
| pposion.<name> | positions of the individual ions in x,y,z, and distance to center, versus time, at intervals commanded by the input parameter jpos |
| pproba.<name> | probabilities of charge states versus time, at time intervals commanded by input parameter jnorms |
| pprojdip.<name> | x, y, z pos of projectile versus time, at time intervals commanded by input parameter jdip |
| prhov.<name> | unused in this version |
| progstatus | Only a flag when dynamics are finished |
| pspenergies.<name> | single particle energies versus time, at time intervals commanded by input parameter jinfo |
| pspvariances.<name> | single particle energy variances versus time, at time intervals commanded by input parameter jinfo |
| pspvariancesp.<name> | single particle energy variances versus time (with correction by projection), at time intervals commanded by input parameter jinfo |
| ptempion.<name> | ion temperatures during ionic-core relaxation |
| pvelion.<name> | ion velocities during ionic-core relaxation, or dynamic calculation with molecular dynamics |
| rsave.<name> | This file contains all parameters of a static convergence to allow for a dynamic start without recomputing the statics: to use it set ismax=0 and istat=1 |
| save.<name> | This file contains all parameters to allow for a dynamic start at time : to use it set irest¿=0 |
| Time | Number of points in the calculation box and used wall time to complete the given number of iterations |

In this table the files that are generated when RTA is activated. I assume this list will be much shorter.

| | |
|---|---|
| `convergenceRTA` | unknown to me, PG? |
| `peqstate` | parameters for convergence of the dtmf process: current iteration number, cycles to convergence, variance, residual err. on density, residual err. on current, parameters mu, muj, energy achieved |
| `prta` | prints at each rta step: time, entropy, laser energy and the mu and temperature of a fermi distribution fitted to the occupation numbers |
| `pspeed.<name>` | prints at each rta step, along x axis, the reference density (spin up and down), achieved density (spin up and down), target x current, achieved x current |

Notes:

- I do not know `<name>.bs`
- I do not know convergenceRTA, maybe this has been added by PG
- pescel, plaser are for any dynamic problem, not only rta, I moved them
- some files are missing, but we have a good start here