Input parameters for the cluster 3D code

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Contents

1 Input files

The cluster 3D code has the following input files:

for005	defines the qualifier `<name>` for the other `for005...` files
for005.`<name>`	general input for settings, static and dynamics
for005ion.`<name>`	ionic configuration of cluster
for005surf.`<name>`	atomic configuration of substrate (optional)

The input for `for005.<name>` is sorted into namelists. They contain:

Namelist GLOBAL	in for005.`<name>`
choice of system	
kxbox	nr. of grid points in x direction
kybox	nr. of grid points in y direction
kzbox	nr. of grid points in z direction
	box sizes must fulfill `kxbox`≥`kybox`≥ `kzbox`
numspin	number of spin components (2=full spin treatment)
	(1=spin averaged, possible problem for ADSIC)
kstate	maximum nr. of s.p. states which is possible (greater than `nclust`)
nclust	number of QM electrons - if set to 0 or a negative value (charge) this will be automatically calculated
	$\texttt{nclust} = \sum_{i=1}^{nion} Z_{ion} = charge$, where Z_{ion} is charge of each ion
nion	number of cluster ions
nspdw	number of spin down electrons
nion2	selects type of ionic background
	$0 \rightarrow$ jellium background
	$1 \rightarrow$ background from ionic pseudo-potentials
	$2 \rightarrow$ background read in from `potion.dat`
radjel	Wigner-Seitz radius of jellium background
surjel	surface thickness of jellium background
bbeta	quadrupole deformation of jellium background
gamma	triaxiality of jellium background
dx,dy,dz,	grid spacing (in Bohr) for the 3D numerical grid - if negative this will be set to an optimal value and a value will be suggested for KXBOX in file NX - the code stops and has to be restarted
	the grid size is defined before compilation in `params.F90`
	it has to be correlant with pseudopotentails
	corresponds to ecut in solid state
imob	global switch to allow ionic motion (if set to 1)
isurf	switch for Ar or MgO surface (isurf=1 activates surface)
iDielec	switch to dielectic support
xDielec	x below which dielectric zone is activated
epsDi	dielectric constant in the dielectric zone
rotclustx,y,z	vector fo angle of initial rotation of ions
temp	electronic temperature in static iteration

Namelist GLOBAL	in for005.<name>

initialization of wave functions	
b2occ	deformation for initial harmonic oscillator wf's
gamocc	triaxiality for initial harmonic oscillator wf's
osfac	factor on initial oscillator radius
deocc	nr. of states above Fermi energy (determines nr. of states)
shiftWFx	shift of initial wavefunctions in x direction
ishiftCMtoOrigin	switch to shift center of mass of cluster to origin
ispinsep	initialize wavefunctiosn with some spin asymmetry
init_lcao	choice of basis for wavefunction initialization
	$=0 \implies$ harmonic oscillator functions (center can be moved by shiftWFx)
	$=1 \implies$ atomic orbitals = WFs centered at ionic sites
itback	nr. of iterations for jellium background

convergence issues	
e0dmp	damping parameter for static solution of Kohn-Sham equations
	(typically about the energy of the lowest bound state)
epswf	step size for static solution of Kohn-Shahm equations (of order of 0.5)
epsoro	required variance to terminate static iteration (order of 10^{-5})
occmix	mixing factor: new (thermal) occupation to old
endcon	requires precision variance, termination criterion

Namelist GLOBAL	in for005.<name>

yet unsorted	
tcoulfalr	switch to FALR Coulomb solver (else exact solver)
dpolx	add stationary dipole field in x-direction
dpoly	add stationary dipole field in y-direction
dpolz	add stationary dipole field in z-direction
scaleclustx	scaling of cluster configuration along x-axis
scaleclusty	scaling of cluster configuration along y-axis
scaleclustz	scaling of cluster configuration along z-axis
scaleclust	if $\neq 1$: scaling of cluster configuration along x-y-z
shiftclustx	shift of cluster configuration along x-axis
shiftclusty	shift of cluster configuration along y-axis
shiftclustz	shioft of cluster configuration along z-axis
iswitch_interpol	switch to interpolated grid for PsP
iplotorbitals	switch to print plot-file pOrbitals for all static states
nproj_states	nr. of electronic states in projectile

QMMM substrate	
idielec	switch to dielectric background
xdielec	distance of dielectric background to lowest GSM layer
epsdi	dielectric constant of dielectric background
isurf	switch to activate dielectric background

Namelist DYNAMIC	in `for005.<name>`
numerical and physical parameters for statics and dynamics	

`dt1`	time step for propagating electronic wavefunctions, $\frac{\Delta t}{\Delta x^2} \leq 1$
`ismax`	maximum number of static iterations
`idyniter`	switch to s.p. energy as E0DMP for 'iter>idyniter'
`ifhamdiag`	diagonalization of m.f. Hamiltonian in static step
	(presently limited to fully occupied configurations)
`isitmax`	nr. of imaginary-time steps to improve static solution
`itmax`	number of time steps for electronic propagation
`ifexpevol`	exponential evolution 4. order instead of TV splitting
`iffastpropag`	accelerated time step in TV splitting
	(for pure electron dynamics, interplay with absorbing b.c. ??)
`irest`	switch to restart dynamics from file 'save'
`istat`	switch to read wavefunctions from file 'rsave'
	it continues static iteration for 'ismax>0'
	it starts dynamics from these wf's for 'ismax=0'
`idenfunc`	choice of density functional for LDA
	$1 \rightarrow$ Perdew & Wang 1992 (default setting)
	$2 \rightarrow$ Gunnarson & Lundquist
	$3 \rightarrow$ only exchange in LDA
`isave`	saves results after every 'isave' steps
	on file 'rsave' in and after static iteration
	on file 'save' in dynamic propagation
`ipseudo`	switch for using pseudo-densities to represent substrate
	atoms
`ipsptype`	type of pseudopotentials: 0 = soft local (errf);
	1 = full Goedecker; 2 = local Goedecker;
	3 = read from file goed.asci (no need to specify) ;
	4 = semicore read from file goed.asci
`directenergy`	`.true.` = direct computation of energy
	(only for `LDA`, `Slater`, `KLI`)
`ifsicp`	selects type of self-interaction correction
	0 = pure LDA, 1 = SIC-GAM, 2 = ADSIC; 3 = SIC-Slater;
	4 = SIC-KLI; 5 = exact exchange; 6 = inactive;
	7 = localized SIC; 8 = full SIC (double set).
	IFSICP=7 or 8 requires switch `twostsic=1` in `define.h`.
	Option IFSICP=7 needs yet testing.
`icooltyp`	type of cooling (0=none, 1=pseudo-dynamics,
	2=steepest descent, 3=Monte Carlo)
`ifredmas`	switch to use reduced mass for ions in dynamics
`ionmdtyp`	ionic propagation (0=none, 1=leap-frog, 2=velocity Verlet)
`ntref`	nr. time step after which absorbing bounds are deactivated
`nabsorb`	number of absorbing points on boundary (0 switches off)
`powabso`	power of absorbing boundary conditions
`ispherabso`	switch to spherical mask in absorbing bounds

Namelist DYNAMIC	in `for005.<name>`

way of excitation	
`centfx`	initial boost of electronic wavefuncftions in x-direction
`centfy`	initial boost of electronic wavefuncftions in y-direction
`centfz`	initial boost of electronic wavefuncftions in z-direction
`shiftinix`	initial x-shift of electronic wavefunctions
`shiftiniy`	initial y-shift of electronic wavefunctions
`shiftiniz`	initial z-shift of electronic wavefunctions
`tempion`	initial temperature of cluster ions
`ekmat`	initial kinetic energy of substrate atom (boost in x, in eV)
`itft`	choice of shape of laser pulse
	1 = ramp laser pulse, sine switching on/off
	2 = gaussian laser pulse
	3 = $\cos^2$ pulse
`tnode`	time (in fs) at which pulse computation starts
`deltat`	length of ramp pulse (`itft = 1`), in fs
`tpeak`	time (in fs, relative to `tnode`) at which peak is reached
	(for `itft = 1` and 2, pulse length becomes 2*`tpeak`)
`omega`	laser frequency (in Ry)
`e0`	laser field strength in Ry/Bohr
`e1x,e1y,e1z`	orientation of pulse
`e0_2`	field strength of second laser pulse (only `itft=3`)
`phase2`	phase of second pulse
`omega2`	frequency of second pulse
`tstart2`	initial ime of second pulse
`tpeak2`	peak time of 2. pulse (pulse length is `2*tpeak2`)
`iexcit`	modus of excitation (0=shifts, 1=rotation)
`iangmo`	switch to compute angular momentum
`irotat`	axis of rotation for excitation (x=1,y=2,z=2,xyz=4)
`phirot`	angle of rotation for excitation (in units of degree)
`phangle`	angle of "rotation" into a $1ph$ state
`phphase`	phase of "rotation" into a $1ph$ state
`nhstate,npstate`	nr. of hole and particle state for $1ph$ excitation
	this $1ph$ option can only be run from `istat=1`
`eproj`	energy of incoming projectile (= last ion in the list)
`vpx,vpy,vpz`	direction of the incoming projectile
`taccel`	time span over which the projectile is accelerated to `eproj`
	for `taccel=0` one has to use `init_lcao=1`

Namelist `DYNAMIC`	in `for005.<name>`
flags for observables	
`iemomsRel`	calculates multipole momentes of electron density relative to origin (0) or c.m. of cluster (1)
`istinf`	modulus for printing information in static iteration
`ifspemoms`	switch to compute and print spatial s.p. moments
`iftransme`	switch to compute and print transition m.elements
`irhoint_time`	modulus for printing slices of integrated densities
`jstinf`	modulus for printing information in dynamic
`jinfo`	modulus for printing dynamical information on `infosp.<name>`
`jdip`	modulus for printing dipole moments on `pdip.<name>`
`jquad`	modulus for printing quadrupole moments on `pquad.<name>`
`jesc`	modulus for printing ionization `pescel.<name>`
`jdiporb`	modulus for printing dipoles for s.p. states on `pdiporb.xyz`
`jenergy`	modulus for printing energy information on `penergies.<name>`
`jener`	modulus for printing ionic energies
`iflocaliz`	activates computation of Becke's localization
`jelf`	modulus for anaylzing and printing electron localization in dynamics various files are written of the form `pelf*.<name>`
`iflocaliz`	modulus for anaylzing and printing electron localization in statics
`jstinf`	modulus for printing s.p. energies and variances
`jpos`	modulus for printing ionic positions on `pposion.<name>`
`jvel`	modulus for printing ionic velocities on `pvelion.<name>`
`jstateoverlap`	switch to compute overlap of static state with the state directly after dynamical initialization
`jforce`	modulus for printing ionic forces
`jgeomion`	modulus for printing global measures of ionic configuration
`jang`	modulus for printing electronic angular momentum
`jangabso`	modulus for printing angular distribution of emitted electrons
`jspdp`	modulus for printing spin dipole momenta
`jposcm`	modulus for printing electronic center of mass
`ipasinf`	modulus for printing information on general observables
`jgeomel`	modulus for printing global measures of electronic geometry
`jelf`	modulus for evaluating an printing electron localization
`jmp`	modulus for storing information for PES
`jnorms`	modulus for printing s.p. norms and ionization probabilities
`jcharges`	modulus for printing radially averaged charge distribution
`drcharges`	radial distance for scanning radially averaged charge distribution
`jplotdensitydiff`	modulus for printing $\rho(t) - \rho(0)$ along x-axis
`jplotdensitydiff2d`	modulus for printing 2D cuts of $\rho(t) - \rho(0)$
`jplotdensity2d`	modulus for printing 2D cuts of density
`jstboostinv`	modulus for evaluating boost-invariant s.p. energy and variance ???
`idenspl`	modulus for printing 2D cuts of density in MTV format ???
`i3dz`	print z-integrated 2D density, following `idenspl` ???
`i3dx`	print x-integrated 2D density, following `idenspl` ???
`i3dstate`	print x- and z-integrated density per state, following `idenspl` ???
`jescmask`	modulus for detailed print of lost electrons ???
`jescmaskorb`	modulus for state-wise detailed print of lost electrons ???

Namelist DYNAMIC		in for00
	yet unsorted	
phi	phase of laser pulse, inactive for electrons, strange for ions ???	
nproj	element number of atomic projectile	
nproj_states	nr. of eletronic states in atomic projectile	
projcharge	charge of ionic projectile	
projvelx	x-velocity of ionic point-charge projectile	
projvely	y-velocity of ionic point-charge projectile	
projvelz	z-velocity of ionic point-charge projectile	
projinix	initial x-coordinate of ionic point-charge projectile	
projiniy	initial y-coordinate of ionic point-charge projectile	
projiniz	initial z-coordinate of ionic point-charge projectile	
modionstep	modulus for ion step (nr. of electron steps per ion step)	
ispidi	=1 switches to initialization by spin-dipole boost	
mxforce	=1 zeroes forces in x-direction for nonlocal PsP ???	
myforce	=1 zeroes forces in y-direction for nonlocal PsP ???	
mzforce	=1 zeroes forces in z-direction for nonlocal PsP ???	
izforcecorr	=1 enforce zero-force condition, =0 tests condition, =-1 disables all	
dinmargin	margin defining inner box in connection with Gaussian pseudo-densities chec	
iangabso	option for origin for angular distribution (1=box, 2=c.m.)	
ipes	activates preparation of measuring points for PES	
nangtheta	number of PAD angular cones in θ direction	
nangphi	number of PAD angular cones in ϕ direction	
delomega	space angle of angular cones in PES check	
angthetal	lower angle θ for PES evaluation	
angthetah	upper angle θ for PES evaluation	
angphil	lower angle ϕ for PES evaluation	
angphih	upper angle ϕ for PES evaluation	
ifreezekspot	=1 freezes KS potential at stage of time=0	
ifixcmion	switch to fix c.m. during ionic motion	
ekin0pp	kinetic energy for initial boost of electrons <u>and</u> ions	
vxn0	boost velocity x-direction relative to ekin0pp	
vyn0	boost velocity y-direction relative to ekin0pp	
vzn0	boost velocity z-direction relative to ekin0pp	
trequest	variable checking CPU time to trigger save operations ??	
timefrac	variable checking CPU time to trigger save operations ??	
nmptheta	number of PES measuring points in θ direction	
nmpphi	number of PES measuring points in ϕ direction	
iscatterelectron	switch to scattering with electron wavepacket	
jattach	modulus to compute attachement probability	
scatterelectronenergy	kinetic energy of impinging electron wavepacket	
scatterelectronvxn	x-velocity of impinging electron wavepacket (relative to scatterelectronen	
scatterelectronvyn	y-velocity of impinging electron wavepacket (relative to scatterelectronen	
scatterelectronvzn	z-velocity of impinging electron wavepacket (relative to scatterelectronen	
scatterelectronx	initial x-coordinate of impinging electron	
scatterelectrony	initial y-coordinate of impinging electron	
scatterelectronz	initial z-coordinate of impinging electron	
scatterelectronw	initial width of impinging electron	

Namelist `DYNAMIC`	in `for005.<name>`
RTA parameters	
`jrtaint`	modulus for invoking RTAS step
`rtamu`	μ parameter for quadratic term on ρ-constraint
`rtamuj`	μ_j parameter for quadratic term on $\mathbf{j}$-constraint
`rtasumvar2max`	criterion for maximal variance of s.p. energies
`rtaeps`	step size in DCMF iteration
`rtae0dmp`	damping energy in DCMF iteration
`rtatempinit`	initial temperature in RTA step
`rtaforcetemperature`	is that really used?
`rtasigee`	effective electron-electron cross section in RTA
`rtars`	effective Wigner-Seitz radius for estimating damping rate

	Namelist SURFACE	in `for005.<name>`
`ne`	Number of fixed shells in substrate	
`nc`	number of O cores in MgO(001)	
`nk`	number of Mg cations in MgO(001)	
`ivdw`	handling of Van-der-Waals with substrate atoms	
	$0 \implies$ no VdW	
	$1 \implies$ enables full computation of VdW	
	$2 \implies$ enables effective VdW through PsP parameters	
`ifadiadip`	switch to adiabatic treatment of substrate dipoles	
`shiftx`	global shift in x for all substrate atoms	
`shifty,shiftz`	as `shiftx` for y and z direction	
`mion`	mass of surface anion (16 for O in MgO(001))	
`mkat`	mass of surface kation (24.3 for Mg in MgO(001))	
`me`	mass of valence shell	
`cspr`	spring constant for interaction between core and valence shell	
`chgc0`	charge of (anion) core	
`chge0`	charge of valence shell	
`chgk0`	charge of cation	
`sigmak`	gauss width of cation	
`sigmac`	gauss width of core	
`sigmav`	gauss width of valence shell	
`iUseCell`	switch for reading/building lattice of substrate atoms	
	$0 \implies$ lattice atoms are read in from input file 'for005surf.*'	
	$1 \implies$ lattice is built from replicating unit cell and	
	lattice parameters `rlattvec` ... are read in (see `md.F`)	
`iPotFixed`	switch for Madelung summation of substrate atoms	
	read/write electrostatic potential from particles with imob=0,	
	so that their run-time calculation can be skipped	
	$0 \implies$ do not read; calculate full potential at each iteration	
	$1 \implies$ read in potFixedIon() from previously prepared file	
	$-1 \implies$ calculate potFixedIon() write result to a file which can	
	be later read in by option 1, stop after that	
	$2 \implies$ calculate potFixedIon() at the beginning, do not write	
`ifmdshort`	includes short range interaction electron–substrate	
`isrtyp(i,j)`	type of interaction between the different kinds of particles	
	$0 \rightarrow$ no short range interaction	
	$1 \rightarrow$ GSM core	
	$2 \rightarrow$ GSM valence shell $=1 \implies$ Born-Mayer type	
	$3 \rightarrow$ GSM kation $=2 \implies$ Argon case	
	$4 \rightarrow$ Na core	
	$5 \rightarrow$ DFT electron	
`unfixCLateralRadx`	radius of cylinder with mobile cores	
`unfixELateralRadx`	radius of cylinder with mobile valence electrons	
`fixCBelowx`	fixes cores which lay below given x value	

Namelist PERIO	in for005.<name>
ch	effective charge of ion
amu	mass of ion in units of hydrogen mass
dr1,dr2	radii of soft local PsP
prho1,prho2	strenghts of soft local PsP
crloc	radius for local part of Goedecker PsP
cc1,cc2	strengths for local part of Goedecker PsP
r0g,r1g,r2g	radii for non-local parts of Goedecker PsP
h0_11g,h0_22g,h0_33g	strenghts for non-local parts of Goedecker PsP
h1_11g,h1_22g,h2_11g	strenghts for non-local parts of Goedecker PsP
radiong	carrier radius for projecteor in non-local Goedecker PsP

Namelist FSIC	in for005.<name>
step	step size in iteration of localizing or symmetry condition
precis	precision in iteration of localizing or symmetry condition
SymUtBegin	nr. iteration where symmetry condition starts
	for pure localizing step set SymUtBegin > ismax
radmaxsym	limiting value in radius division for actucal step

Ionic structure and e^--initialization in for005ion.<name>	
	This initialization does not use NAMELIST but reads input in fixed order.
	Each line stands for one ion. Each column has a definite meaning.
Col. 1	x-coordinate
Col. 2	y-coordinate
Col. 3	z-coordinate
Col. 4	number of element in periodic system (e.g.: Na↔11)
Col. 5	only init_lcao=1: ordering of nodes in repeated initialization at this ion
Col. 6	only init_lcao=1: radius of initial Gaussian at this ion
Col. 7	only init_lcao=1: starting spin for initalization at this ion

The handling of the initialization of electronic wavefunctions is rather involved. A more detailed explanation is given in appendix A.

A On the initialization of the electronic wavefunctions

The basic switch is `init_lcao`. The case `init_lcao=0` is the simpler option. This initializes harmonic oscillator wavefunctions about one common center. This center is usually the origin of the coordinte-space grid. It can be moved deliberately by `shiftWFx`, `shiftWFy`, and `shiftWFz`. The initial oscillator may be deformed. Its deformation is given by the dimensionless quadrupole `b2occ` and triaxiality `gamocc` (in degree). The oscillator states are filled in order of increasing oscillator energies. A spin asymmtry can be enforced with `ispinsep=1`. This option is useful when dealing with odd electron number. The upper end of initialization is determined by `deocc`. A `deocc` ≈ 0 typically initializes just as many states as are occupied. If more is required, enhance `deocc`.

The case `init_lcao=1` initializes wavefunctions which are localized at the ions. This option is richer and a bit hard to handle. In a first step, the total number of wavefunctions is estimated and it is computed how many wavefunctions have to be initialized then for each ion. At one given ion, initialization starts with the $1s$ oscillator state. The first choice of spin is taken from column 7 of `for005ion.<name>` which initializes the entry of the actual ion in the the `ipol` array. The value `ipol=+1` sets a spin up (i.e. `ispin=1` in the code) as the first choice, while `ipol=-1` sets a spin down (i.e. `ispin=2`). If more than one state is to be occupied, the next is then the $1s$ state with opposite spin. Next comes the $1p_i$ state with first spin where i is the direction given as first entry in column 5. For example if column 5 selects 'yzx', the $1p_y$ comes here. Occupation continues in order given by column 5 and 7 until the wanted number of orbitals at this ion site is reached. Column 6 sets the oscillator radius for the initialization at this ion (which allows to deal efficiently with systems consisting of very different ions). Column 7 becomes important for ions associated with an odd number of electrons as, e.g., hydrogen. One ought to distribute an equal collection of spins up and down over the whole system to avoid unnaturally polarized molecules.