Input parameters for the cluster 3D code

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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
	`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 → jellium background
	1 → background from ionic pseudo-potentials
	2 → 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
	$=0 \Longrightarrow$ harmonic oscillator functions (center can be moved by `shiftWFx`)
	$=1 \Longrightarrow$ 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 → Perdew & Wang 1992 (default setting) 2 → Gunnarson & Lundquist 3 → 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

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 ???

Namelist DYNAMIC	in for005.<name>
yet unsorted	
phi	phase of laser pulse, inactive for electrons, strange for ions ???
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 check default
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
nmptheta	number of PES measuring points in θ direction
nmpphi	number of PES measuring points in ϕ direction

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 **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 `EXTENSIONS`	in `for005.<name>`
extended options (not to appear in public version)	
`trequest`	variable checking CPU time to trigger save operations
`timefrac`	variable checking CPU time to trigger save operations
`iscatterelectron`	switch to scattering with electron wavepacket
`jattach`	modulus to compute attachement probability
`scatterelectronenergy`	kinetic energy of impinging electron wavepacket
`scatterelectronvxn`	x-velocity of electron wavepacket (relative to energy)
`scatterelectronvyn`	y-velocity of electron wavepacket (relative to energy)
`scatterelectronvzn`	z-velocity of electron wavepacket (relative to energy)
`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
`jescmask`	modulus for detailed print of lost electrons
`jescmaskorb`	modulus for state-wise detailed print of lost electrons
`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`
`nproj`	element number of atomic projectile
`nproj_states`	nr. of eletronic states in atomic projectile

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
	$0 \Longrightarrow$ no VdW
	$1 \Longrightarrow$ enables full computation of VdW
	$2 \Longrightarrow$ 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
	$0 \Longrightarrow$ lattice atoms are read in from input file 'for005surf.*'
	$1 \Longrightarrow$ 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
	$0 \Longrightarrow$ do not read; calculate full potential at each iteration
	$1 \Longrightarrow$ read in potFixedIon() from previously prepared file
	-1 $\Longrightarrow$ calculate potFixedIon() write result to a file which can be later read in by option 1, stop after that
	$2 \Longrightarrow$ 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 $=1 \Longrightarrow$ Born-Mayer type
	$3 \rightarrow$ GSM kation $=2 \Longrightarrow$ 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` $\approx$ `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.