Namelist input parameters for the cluster 3D code

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These notes serve to explain the input structure of the cluster/molecule 3D code. It explains the full capabilities of the code. We want to publish only a subset. All options addressed in namelist `EXTENSIONS`, `FSIC2`, and `SURFACE` should not appear in the public version. The switches to these parts are immersed in the code with preproccesor variables `extended`, `fsic`, and `raregas`. We should keep the code in the repository always in its complete version and write a little piece of software which reads the source files and produces new sources without the line enclosed be the `#if(extended)`, `#if(extended)`, and `#if(raregas)` closures.
Note also the old input files have to changed. The namelist "&EXTENSIONS" has to follow namelist "&DYNAMIC" and all non-public input parameters have to be moved to there. Moreover, The namelist "&FSIC" has to renamed "&FSIC2". A few examples with input in old style are collected in the directory `examples` while examples with input in new style com in `samples`.

The input is arranged in the following three 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 Fortran namelists. The following tables list all input variables entered through these namelists and gives a short explanation. Comments and issues for development are marked in red. A mere ??? indicates a variable which should be considered to be shifted to namelist `extension`.

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	
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	
tcoulfalr	switch to FALR Coulomb solver (else exact solver)	
iswitch_interpol	switch to interpolated grid for PsP	
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	
nion2	selects type of ionic background	
	0 → jellium background	
	1 → background from ionic pseudo-potentials	
	2 → background read in from potion.dat	
temp	electronic temperature in static iteration	
nion	number of cluster ions	
nspdw	number of spin down electrons	
radjel	Wigner-Seitz radius of jellium background	
surjel	surface thickness of jellium background	
bbeta	quadrupole deformation of jellium background	
gamma	triaxiality of jellium background	
itback	nr. of iterations for jellium background	
rotclustx,y,z	vector fo angle of initial rotation of ions	
scaleclustx	scaling of ionic configuration along x-axis	
scaleclusty	scaling of ionic configuration along y-axis	
scaleclustz	scaling of ionic configuration along z-axis	
scaleclust	if $\neq 1$: scaling of ionic configuration along x-y-z	
shiftclustx	shift of ionic configuration along x-axis	
shiftclusty	shift of ionic configuration along y-axis	
shiftclustz	shift of ionic configuration along z-axis	

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 of box	
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	
	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 to be sorted	
dpolx	add stationary dipole field in x-direction (better placed in dynamic?)	
dpoly	add stationary dipole field in y-direction (better placed in dynamic?)	
dpolz	add stationary dipole field in z-direction (better placed in dynamic?)	

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. 7 = localized SIC, 8 = full SIC (real), 9 = full SIC(complex) in extended branch fsic	
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) (Should we move "leap-frog" to the extended version???)	
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)
nhstate,npstate	nr. of hole and particle state for 1ph excitation
	this option can only be run from istat=1
phangle	angle of "rotation" into a 1ph state
phphase	phase of "rotation" into a 1ph state
	phangle and phphase must be different, ideally phangle-phphase=90

Namelist DYNAMIC	in for005.<name>
flags for observables	
iplotorbitals	switch to print plot-file pOrbitals for all static states
iemomsRel	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 general information along dynamics
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

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	
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 and 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
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
jstboostinv	modulus for evaluating boost-invariant s.p. energy and variance

Namelist SURFACE	in for005.<name>
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
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$\leftrightarrow$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