Octopus: structure of the code

Martin Lüders

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Overview

- General structure of the code
- Structure of a calculation: GS and TD
- Real-space representation: and mesh functions and operators
- Multisystems: systems and interactions
- Time propagation

Introduction

Code refactoring:

- big changes to the code, while keeping the code functional

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This talk: Representation strongly simplified

The global structure

General code structure

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  - I/O: reading and writing data

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    - `*_init()`:

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- Most components have `*_init()` and `*_end()` routines.
  - `*_init()`:
    - initialize data structures
    - read related input variables
  - `*_end()`:
    - clean up: release memory

General code structure

Example: the main routine:

```
program main

  [...]

  !  start code components

  call global_init()               ! initialize the mpi, clocks, etc.
  call parser_init()               ! initialize the input parser
  call messages_init()             ! initialize the message system
  call walltimer_init()            ! initialize the timer module
  call io_init()                   ! initialize the I/O subsystem
  call calc_mode_par_init()        ! initialize parallelization strategy
  call profiling_init()            ! initialize and start the profiling system

  call run(inp_calc_mode)          ! pass control to the 'actual code' running the calculation

  !  stop code components

  call profiling_end()
  call calc_mode_par_end()
  call io_end()
  call walltimer_end()
  call messages_end()
  call parser_end()
  call global_end()

end program
```

General code structure: Directory structure

What you find in the package:

`build`	related to build system
`doc`	Documentation, manuals, tutorials
`external_libs`	external libraries shipped with Octopus
`liboct_parser`	the input parser library
`m4`	m4 macros for autotools
`scripts`	some analysis scripts
`share`	pseudopotentials, GPU kernels, recipes, etc.
`src`	our octopus lives here
`testsuite`	test files and input files for the tests

...

General code structure: Directory structure

Content of `src/`:

`basic`	general routines
`basis_set`	atomic orbitals
`classical`	classical particle classes
`common-rules.make`	
`dftbplus`	interface to DFTB+
`electrons`	all related to electrons
`fdep`	(helper script for automake)
`grid`	grid, mesh, etc.
`hamiltonian`	Hamiltonain (general, but also electronic, e.g.projectors, v_xc)
`include`	macro definitions
`interactions`	interaction classes
`ions`	ions, boxes, symmetries
`main`	main routines
`Makefile.am`	
`Makefile.in`	

General code structure: Directory structure

Content of `src/`:

`math`	mathematical routines, interfaces to blas, fftw, etc.
`maxwell`	All about Maxwell
`multisystem`	The multisystem framework (propagator class)
`opt_control`	optimal control
`output`	the output module
`poisson`	the Poisson solver and interface to PSOLVER library
`scf`	SCF cycle: LCAO, convergence criteria, mixer
`species`	mainly pseudopotentials
`states`	wave functions, density, etc.
`sternheimer`	linear response
`td`	propagators (old formalism)
`utils`	external utilities

General code structure: Directory structure

Files in the `src/main/` folder:

```
casida.F90
casida_inc.F90
geom_opt.F90
ground_state.F90
invert_ks.F90
main.F90
phonons_fd.F90
pulpo.F90
run.F90
static_pol.F90
system_factory.F90
test.F90
time_dependent.F90
```

General code structure

Common objects

`gr`	The object containing the grid and mesh
`space`	Description of the periodicity and dimensionality
`st`	The states (i.e. wave functions for electrons)
`hm`	The Hamiltonian
`scf`	An object containing information about the SCF cycle
`td`	An object containing information about time-dependent runs

How a calculation works...

The calculation modes

gs	Calculation of the ground state.
unocc	Calculation of unoccupied/virtual KS states. Can also be used for a non-self-consistent calculation of states at arbitrary k-points, if density.obf from gs is provided in the restart/gs directory.
td	Time-dependent calculation (experimental for periodic systems).
go	Optimization of the geometry.
opt_control	Optimal control.
em_resp	Calculation of the electromagnetic response: electric polarizabilities and hyperpolarizabilities and magnetic susceptibilities (experimental for periodic systems).
casida	Excitations via Casida linear-response TDDFT; for finite systems only.
vdw	Calculate van der Waals coefficients.
vib_modes	Calculation of the vibrational modes.
invert_ks	Invert the Kohn-Sham equations (experimental).
recipe	Prints out a tasty recipe.
...	and others

The calculation modes

The `run()` routine:

```
subroutine run(cm):
  integer, intent(in) :: cm
  ...
  select case (calc_mode_id)
  case (OPTION__CALCULATIONMODE__GS)                ! ground state
    call ground_state_run(systems, from_scratch)
  case (OPTION__CALCULATIONMODE__UNOCC)             ! unoccupied states
    call unocc_run(systems, from_scratch)
  case (OPTION__CALCULATIONMODE__TD)                ! time propagation
    call time_dependent_run(systems, from_scratch)
  case (OPTION__CALCULATIONMODE__GO)                ! geometry optimization
    call geom_opt_run(systems, from_scratch)
  ...
  end select
  ...
end subroutine run
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    call geom_opt_run(systems, from_scratch)
  ...
  end select
  ...
end subroutine run
```

Concentrate on:

- Ground state calculation
- Time propagation

Ground state calculation (electrons only)

- Startup:
  - initial wave functions:
    - Restart
    - LCAO from diagonalized speudo-wavefunctions
    - random wave functions
  - setup initial Hamiltonian

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  - update Hamiltonian
  - check convergence criteria

Ground state calculation (electrons only)

(simplified) SCF cycle: (`scf/scf.F90`)

```
    do iter = 1, scf%max_iter
```

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do iter = 1, scf%max_iter
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do iter = 1, scf%max_iter
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  call eigensolver_run(scf%eigens, namespace, gr, st, hm, iter)
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  call density_calc(st, gr, st%rho)
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  call energy_calc_total(namespace, space, hm, gr, st, iunit = 0)
  call mixing(scf%smix)
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Ground state calculation (electrons only)

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- Matrix is huge and sparse: no direct diagonalization
- Iterative schemes:
  - Conjugate gradient: (`cg`, `cg_new`)
  - Pre-conditioned Lanczos (`plan`)
  - Residual minimization scheme, direct inversion in the iterative subspace (`rmmdiis`)

Time-dependent calculations (for electrons)

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- different ways to approximate
  - the integration
    - `TDPropagator` for electrons
    - `TDSystemPropagator` for multisystem framework
  - the exponential
    - `TDExponentialMethod`

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- still different implementations for matter (electrons + ions) and the multisystem approach (more on new approach later)
- this will change soon...

The grid

Real-space grid

The grid describes a number of things:

- the mesh (the actual points in space)
- the simulation box (region of space over which the mesh extends)
- the derivatives
- the stencil

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- the stencil

```
type grid_t
  ! Components are public by default
  type(simul_box_t)                    :: sb
  type(mesh_t)                         :: mesh
  type(derivatives_t)                  :: der
  class(coordinate_system_t), pointer :: coord_system
  type(stencil_t)                      :: stencil
  type(symmetries_t)                   :: symm
end type grid_t
```

Real-space grid

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- can be distributed over processes (domain decomposition)
- access via linear indices (local and global index)
- We need some 'extra points':
  - for boundary conditions:
    functions on these points are not updated
  - halo points (ghost points):
    when using domain decompositions, each process needs access to neighboring domains.

Real-space grid

Memory layout:

- mesh sizes:

Real-space grid

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  `np` number of local 'inner' points

Real-space grid

Memory layout:

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`np`	number of local 'inner' points
`np_part`	number of local 'inner' points + 'ghost' points + boundary points

Real-space grid

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- mesh sizes:

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`np_part`	number of local 'inner' points + 'ghost' points + boundary points
`np_global`	number of global 'inner' points

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`np_part_global`	number of global 'inner' points + boundary points

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`np_part_global`	number of global 'inner' points + boundary points

- ordering:

Real-space grid

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`np_part_global`	number of global 'inner' points + boundary points

- ordering:
  - inner points first `[1:np]`

Real-space grid

Memory layout:

- mesh sizes:

`np`	number of local 'inner' points
`np_part`	number of local 'inner' points + 'ghost' points + boundary points
`np_global`	number of global 'inner' points
`np_part_global`	number of global 'inner' points + boundary points

- ordering:
  - inner points first `[1:np]`
  - ghost and boundary points: `[np+1:np_part]`

Real-space grid

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- ordering:
  - inner points first `[1:np]`
  - ghost and boundary points: `[np+1:np_part]`
- mesh points: `mesh%x(1:mesh%np_part, 1:space%dim)`

Real-space grid

Mesh functions:

- position dependent quantities are stored as so-called mesh functions.

Real-space grid

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- Examples:

  `rho(1:gr%mesh%np, 1:st%d%nspin)` (no ghost points needed here)

  `hm%vhartree(1:gr%mesh%np_part)`

  `hm%a_ind(1:gr%mesh%np_part, 1:space%dim)`

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Operations on mesh functions:

- local operations: point-wise operation, simple loop
- integrations: summation in each domain and reduction over domains
- derivatives: need to consider ghost and boundary points

Real-space grid

Pre-defined operations on mesh functions:

dot product `X(mf_dotp)(mesh, f1, f2, reduce, dotu, np)`

Real-space grid

Pre-defined operations on mesh functions:

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Real-space grid

Pre-defined operations on mesh functions:

dot product	`X(mf_dotp)(mesh, f1, f2, reduce, dotu, np)`
norm	`X(mf_nrm2)(mesh, ff, reduce)`
Laplacian	`X(derivatives_lapl)(der, ff, op_ff, ghost_update, set_bc, factor)`

Real-space grid

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Real-space grid

Pre-defined operations on mesh functions:

dot product	`X(mf_dotp)(mesh, f1, f2, reduce, dotu, np)`
norm	`X(mf_nrm2)(mesh, ff, reduce)`
Laplacian	`X(derivatives_lapl)(der, ff, op_ff, ghost_update, set_bc, factor)`
gradient	`X(derivatives_grad)(der, ff, op_ff, ghost_update, set_bc)`

However: We are trying to use batches wherever possible.

Batches

- often one has to operate on many mesh functions at once (e.g. wave functions)

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- excerpt from `batch_t`:

```
!> unpacked variables; linear variables are pointers with different shapes
FLOAT, pointer, contiguous,     public :: dff(:, :, :)
CMPLX, pointer, contiguous,     public :: zff(:, :, :)
FLOAT, pointer, contiguous,     public :: dff_linear(:, :)
CMPLX, pointer, contiguous,     public :: zff_linear(:, :)
!> packed variables; only rank-2 arrays due to padding to powers of 2
FLOAT, pointer, contiguous,     public :: dff_pack(:, :)
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- basic math operations implemented for batches
- more in upcoming lectures.

Operators and obervables

Calculating expectation values:

- operators can be expressed in terms of defined math operations
- many terms already implemented in the Hamiltonian
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Let's look at some code: contributions to the total energy (`electrons/energy_calc.F90`)

```
subroutine energy_calc_total(namespace, space, hm, gr, st, iunit, full)

FLOAT function X(energy_calc_electronic)(namespace, hm, der, st, terms) result(energy)

subroutine X(calculate_expectation_values)(namespace, hm, der, st, eigen, terms)
```

Operators and obervables

```
subroutine energy_calc_total(namespace, space, hm, gr, st, iunit, full)

type(namespace_t),        intent(in)    :: namespace
type(space_t),            intent(in)    :: space
type(hamiltonian_elec_t), intent(inout) :: hm
type(grid_t),             intent(in)    :: gr
type(states_elec_t),      intent(inout) :: st
integer, optional,        intent(in)    :: iunit
logical, optional,        intent(in)    :: full

  ...

hm%energy%eigenvalues = states_elec_eigenvalues_sum(st)

if (full_ .or. hm%theory_level == HARTREE .or. hm%theory_level == HARTREE_FOCK &
  .or. hm%theory_level == GENERALIZED_KOHN_SHAM_DFT) then

  if (states_are_real(st)) then
    hm%energy%kinetic = denergy_calc_electronic(namespace, hm, gr%der, st, terms=TERM_KINETIC)
    hm%energy%extern_local = denergy_calc_electronic(namespace, hm, gr%der, st, terms=TERM_LOCAL_EXTERNAL)
    hm%energy%extern_non_local = denergy_calc_electronic(namespace, hm, gr%der, st, &
                                                         terms=TERM_NON_LOCAL_POTENTIAL)
    hm%energy%extern = hm%energy%extern_local + hm%energy%extern_non_local
  else
  ... ! same with z prefix
  end if

end if
```

Operators and obervables

```
FLOAT function X(energy_calc_electronic)(namespace, hm, der, st, terms) result(energy)

  type(namespace_t),        intent(in)    :: namespace
  type(hamiltonian_elec_t), intent(in)    :: hm
  type(derivatives_t),      intent(in)    :: der
  type(states_elec_t),      intent(inout) :: st
  integer,                  intent(in)    :: terms

  R_TYPE, allocatable  :: tt(:, :)

  PUSH_SUB(X(energy_calc_electronic))

  SAFE_ALLOCATE(tt(st%st_start:st%st_end, st%d%kpt%start:st%d%kpt%end))

  call X(calculate_expectation_values)(namespace, hm, der, st, tt, terms = terms)

  energy = states_elec_eigenvalues_sum(st, TOFLOAT(tt))

  SAFE_DEALLOCATE_A(tt)
  POP_SUB(X(energy_calc_electronic))

end function X(energy_calc_electronic)
```

Operators and obervables

```
subroutine X(calculate_expectation_values)(namespace, hm, der, st, eigen, terms)

  type(namespace_t),        intent(in)    :: namespace
  type(hamiltonian_elec_t), intent(in)    :: hm
  type(derivatives_t),      intent(in)    :: der
  type(states_elec_t),      intent(inout) :: st
  R_TYPE,                   intent(out)   :: eigen(st%st_start:, st%d%kpt%start:) !< (:st%st_end, :st%d%kpt%end
  integer, optional,        intent(in)    :: terms

  integer :: ik, minst, maxst, ib
  type(wfs_elec_t) :: hpsib

  do ik = st%d%kpt%start, st%d%kpt%end
    do ib = st%group%block_start, st%group%block_end

      minst = states_elec_block_min(st, ib)
      maxst = states_elec_block_max(st, ib)

      call st%group%psib(ib, ik)%copy_to(hpsib)
      call X(hamiltonian_elec_apply_batch)(hm, namespace, der%mesh, st%group%psib(ib, ik), hpsib, terms = terms
      call X(mesh_batch_dotp_vector)(der%mesh, st%group%psib(ib, ik), hpsib, eigen(minst:maxst, ik), reduce = .
      call hpsib%end()

    end do
  end do

  if (der%mesh%parallel_in_domains) call der%mesh%allreduce(&
    eigen(st%st_start:st%st_end, st%d%kpt%start:st%d%kpt%end))

end subroutine X(calculate_expectation_values)
```

Operators and obervables

in `hamiltonian/hamiltonian_elec_inc.F90`:

```
subroutine X(hamiltonian_elec_apply_batch) (hm, namespace, mesh, psib, hpsib, terms, set_bc)

  ...

  if (bitand(TERM_KINETIC, terms_) /= 0) then
    ASSERT(associated(hm%hm_base%kinetic))
    call profiling_in(prof_kinetic_start, TOSTRING(X(KINETIC_START)))
    call X(derivatives_batch_start)(hm%hm_base%kinetic, hm%der, epsib, hpsib, handle, &
                                    set_bc = .false., factor = -M_HALF/hm%mass)
    call profiling_out(prof_kinetic_start)
  end if

  ...

  if (bitand(TERM_KINETIC, terms_) /= 0) then
    call profiling_in(prof_kinetic_finish, TOSTRING(X(KINETIC_FINISH)))
    call X(derivatives_batch_finish)(handle)
    call profiling_out(prof_kinetic_finish)
  else
    call batch_set_zero(hpsib)
  end if
```

Operators and obervables

in `hamiltonian/hamiltonian_elec_inc.F90`:

```
subroutine X(hamiltonian_elec_apply_batch) (hm, namespace, mesh, psib, hpsib, terms, set_bc)

  ...

  if (bitand(TERM_KINETIC, terms_) /= 0) then
    ASSERT(associated(hm%hm_base%kinetic))
    call profiling_in(prof_kinetic_start, TOSTRING(X(KINETIC_START)))
    call X(derivatives_batch_start)(hm%hm_base%kinetic, hm%der, epsib, hpsib, handle, &
                                    set_bc = .false., factor = -M_HALF/hm%mass)
    call profiling_out(prof_kinetic_start)
  end if

  ...

  if (bitand(TERM_KINETIC, terms_) /= 0) then
    call profiling_in(prof_kinetic_finish, TOSTRING(X(KINETIC_FINISH)))
    call X(derivatives_batch_finish)(handle)
    call profiling_out(prof_kinetic_finish)
  else
    call batch_set_zero(hpsib)
  end if
```

split in start and finish routine to enable other operations during communication.

Output

Calculations are a (huge!) waste of time...

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... if we are not writing out the results.

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... if we are not writing out the results.

Modules to write out data:

- file output:
    - larger amounts of data
    - not intended for standard out
- messages: everything for stdout and stderr
    - Information
    - Warnings
    - Error messages

Data output

Distinguish between

- mesh data:
  - Examples: density $n(\vec{r})$, fields $\vec{E}(\vec{r})$, wave functions $\phi_i(\vec{r})$
  - handled by `output_oct_m` and `io_oct_m`.
  - also used when these functions are time-dependent.

Data output

Distinguish between

- mesh data:
  - Examples: density $n(\vec{r})$, fields $\vec{E}(\vec{r})$, wave functions $\phi_i(\vec{r})$
  - handled by `output_oct_m` and `io_oct_m`.
  - also used when these functions are time-dependent.
- time-dependent functions (scalar or vectors, but no fields)
  - Examples: total energy $E(t)$, magtetization $\vec{m}(t)$
  - handled by `td_write_m`

Data output

Mesh data: `output_oct_m` and `io_oct_m`:

- `output/output.F90: output_init(outp, namespace, space, st, nst, ks)`:
  - parse `output` variable
    (via `io_function_read_what_how_when()`; new output options need to be implemented here.)
  - parse other output related input variables

Data output

Mesh data: `output_oct_m` and `io_oct_m`:

- `output/output.F90: output_init(outp, namespace, space, st, nst, ks)`:
  - parse output variable (via `io_function_read_what_how_when()`; new output options need to be implemented here.)
  - parse other output related input variables
- `output/output.F90: output_all(outp, namespace, space, dir, gr, ions, iter, st, hm, ks)`:
  - is automatically called at end of SCF (or similar) calculation, or at specified iteration intervals.
  - calls specific output routines, if requested. (e.g. `output_states()`)

Data output

What, how and when to write?

- mesh data:
  From grid/io_function.F90:

```
subroutine io_function_read_what_how_when(namespace, space, what, how, output_interval, &
                                          what_tag_in, how_tag_in, output_interval_tag_in, ignore_error)

  type(namespace_t), intent(in)          :: namespace
  type(space_t),     intent(in)          :: space
  logical,           intent(inout)       :: what(MAX_OUTPUT_TYPES)    !> which quantities?
  integer(8),        intent(out)         :: how(0:MAX_OUTPUT_TYPES)   !> output format
  integer,           intent(out)         :: output_interval(0:MAX_OUTPUT_TYPES)
  character(len=*),  optional, intent(in) :: what_tag_in
  character(len=*),  optional, intent(in) :: how_tag_in
  character(len=*),  optional, intent(in) :: output_interval_tag_in
  logical, optional, intent(in)          :: ignore_error   !> Ignore error check.
                                                           !> Used when called from some external utili
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Data output

What, how and when to write?

- mesh data:
  From grid/io_function.F90:

```
subroutine io_function_read_what_how_when(namespace, space, what, how, output_interval, &
                                          what_tag_in, how_tag_in, output_interval_tag_in, ignore_error)

  type(namespace_t), intent(in)          :: namespace
  type(space_t),     intent(in)          :: space
  logical,           intent(inout)       :: what(MAX_OUTPUT_TYPES)    !> which quantities?
  integer(8),        intent(out)         :: how(0:MAX_OUTPUT_TYPES)   !> output format
  integer,           intent(out)         :: output_interval(0:MAX_OUTPUT_TYPES)
  character(len=*),  optional, intent(in) :: what_tag_in
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  logical, optional, intent(in)          :: ignore_error   !> Ignore error check.
                                                           !> Used when called from some external utili
```

- time-dependent functions:
  From grid/io_function.F90:

```
subroutine td_write_init(writ, namespace, space, outp, gr, st, hm, ions, ks, ions_move, &
                         with_gauge_field, kick, iter, max_iter, dt, mc)
```

Data output

Example: Output of a the density

From `output/output_states_inc.F90`:

```
subroutine output_states(outp, namespace, space, dir, st, gr, ions, hm, iter)

  ...

  if (outp%what_now(OPTION__OUTPUT__DENSITY, iter)) then
    fn_unit = units_out%length**(-space%dim)
    do is = 1, st%d%nspin
      if (st%d%nspin == 1) then
        write(fname, '(a)') 'density'
      else
        write(fname, '(a,i1)') 'density-sp', is
      end if
      call dio_function_output(outp%how(OPTION__OUTPUT__DENSITY), &
                               dir, fname, namespace, space, gr%mesh, &
                               st%rho(:, is), fn_unit, ierr, ions = ions, &
                               grp = st%dom_st_kpt_mpi_grp)
    end do
  end if
```

Data output

Example: Output of a mesh function

From grid/io_functions_inc.F90:

```
subroutine X(io_function_output) (how, dir, fname, namespace, space, mesh, ff, unit, &
                                  ierr, ions, grp, root, is_global)

  integer(8),                   intent(in)  :: how         !< output format descriptor
  character(len=*),             intent(in)  :: dir         !< directory
  character(len=*),             intent(in)  :: fname       !< filename
  type(namespace_t),            intent(in)  :: namespace   !< namespace
  type(space_t),                intent(in)  :: space
  type(mesh_t),                 intent(in)  :: mesh
  R_TYPE,             target,   intent(in)  :: ff(:)       !< mesh function to be printed
  type(unit_t),                 intent(in)  :: unit        !< output units
  integer,                      intent(out) :: ierr
  type(ions_t),       optional, intent(in)  :: ions
  type(mpi_grp_t),    optional, intent(in)  :: grp         !< the group that shares the same data,
                                                           !< must contain the domains group
  integer,            optional, intent(in)  :: root        !< which process is going to write the data
  logical,            optional, intent(in)  :: is_global   !< Input data is mesh%np_global?
                                                           !< And, thus, it has not be gathered
```

This routine deals with domain parallelization.

Messages: Info, Warnings, Errors

Implemented in `messages_oct_m`:

- several functions to write messages

Messages: Info, Warnings, Errors

Implemented in `messages_oct_m`:

- several functions to write messages
    - `messages_info(no_lines, iunit, verbose_limit, stress, all_nodes)` writes information, and can be controlled by verbose-level.

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Implemented in `messages_oct_m`:

- several functions to write messages
  - `messages_info(no_lines, iunit, verbose_limit, stress, all_nodes)`
    writes information, and can be controlled by verbose-level.
  - `messages_warning(no_lines, all_nodes, namespace)`
    writes warnings (independent of verbose level)
    code continues

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  - `messages_warning(no_lines, all_nodes, namespace)`
    writes warnings (independent of verbose level)
    code continues
  - `messages_fatal(no_lines, only_root_writes, namespace)`
    writes fatal error message
    stops the code.

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- provides (global) `message` array

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    writes warnings (independent of verbose level)
    code continues
  - `messages_fatal(no_lines, only_root_writes, namespace)`
    writes fatal error message
    stops the code.
- provides (global) `message` array
- handles parallelism

Messages: Info, Warnings, Errors

Examples:

- Info

```
write(message(1), '(a, i4, a)') 'Info: SCF converged in ', iter, ' iterations'
write(message(2), '(a)')        ''
call messages_info(2)
```

Messages: Info, Warnings, Errors

Examples:

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write(message(2), '(a)')        ''
call messages_info(2)
```

- Warning

```
if (ierr /= 0) then
  message(1) = 'Unable to write mixing information.'
  call messages_warning(1)
end if
```

Messages: Info, Warnings, Errors

Examples:

- Info

```
write(message(1), '(a, i4, a)') 'Info: SCF converged in ', iter, ' iterations'
write(message(2), '(a)')        ''
call messages_info(2)
```

- Warning

```
if (ierr /= 0) then
  message(1) = 'Unable to write mixing information.'
  call messages_warning(1)
end if
```

- Error

```
select type (system)
class is (multisystem_basic_t)
  message(1) = "CalculationMode = gs not implemented for multi-system calculations"
  call messages_fatal(1)
type is (electrons_t)
  call ground_state_run_legacy(system, from_scratch)
end select
```

Multisystems

The multisystem framework

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- allow calculation of coupled systems

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- Examples of systems:

Multisystems

The multisystem framework

- allow calculation of coupled systems
- Examples of systems:
    - maxwell

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- Examples of systems:
  - maxwell
  - classical particles

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- Examples of systems:
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    - charged particles

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- allow calculation of coupled systems
- Examples of systems:
  - maxwell
  - classical particles
  - charged particles
  - ions

Multisystems

The multisystem framework

- allow calculation of coupled systems
- Examples of systems:
  - maxwell
  - classical particles
  - charged particles
  - ions
  - electrons

Multisystems

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- allow calculation of coupled systems
- Examples of systems:
  - maxwell
  - classical particles
  - charged particles
  - ions
  - electrons
  - tight binding model

Multisystems

The multisystem framework

- allow calculation of coupled systems
- Examples of systems:
    - maxwell
    - classical particles
    - charged particles
    - ions
    - electrons
    - tight binding model
    - etc.

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- use object oriented approach!

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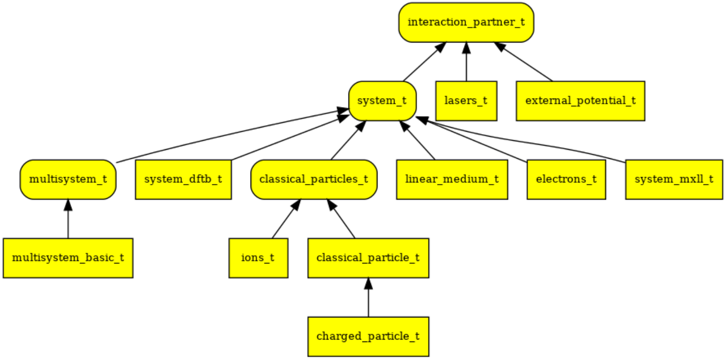
  - classical particles
  - charged particles
  - ions
  - electrons
  - tight binding model
  - etc.
- re-use as much code as possible between different systems
- use object oriented approach!
- represent systems as classes and use inheritance

System classes

Currently implemented system classes:



Rounded boxes: abstract class
Arrows indicate inheritance.

System classes

The abstract class `interaction_partner_t`:

```
type, abstract :: interaction_partner_t
private
  type(namespace_t), public :: namespace
  type(clock_t),     public :: clock
  type(space_t),     public :: space

  type(integer_list_t), public :: supported_interactions_as_partner

  type(quantity_t),  public :: quantities(MAX_QUANTITIES) !< Array of all possible quantities.
                                                          !< The elements of the array are accessed using the
                                                          !< quantity‘s identifiers.
contains
  procedure(interaction_partner_update_exposed_quantities),     deferred :: update_exposed_quantities
  procedure(interaction_partner_update_exposed_quantity),       deferred :: update_exposed_quantity
  procedure(interaction_partner_init_interaction_as_partner),   deferred :: init_interaction_as_partner
  procedure(interaction_partner_copy_quantities_to_interaction), deferred :: copy_quantities_to_interaction
end type interaction_partner_t
```

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  procedure(interaction_partner_init_interaction_as_partner),   deferred :: init_interaction_as_partner
  procedure(interaction_partner_copy_quantities_to_interaction), deferred :: copy_quantities_to_interaction
end type interaction_partner_t
```

- abstract class: cannot be instantiated

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private
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  type(clock_t),     public :: clock
  type(space_t),     public :: space

  type(integer_list_t), public :: supported_interactions_as_partner

  type(quantity_t),  public :: quantities(MAX_QUANTITIES) !< Array of all possible quantities.
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  procedure(interaction_partner_update_exposed_quantity),        deferred :: update_exposed_quantity
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  procedure(interaction_partner_copy_quantities_to_interaction), deferred :: copy_quantities_to_interaction
end type interaction_partner_t
```

- abstract class: cannot be instantiated
- defines basic variables and interface for all classes which can be partner in an interaction

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  type(namespace_t), public :: namespace
  type(clock_t),     public :: clock
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  procedure(interaction_partner_copy_quantities_to_interaction), deferred :: copy_quantities_to_interaction
end type interaction_partner_t
```

- abstract class: cannot be instantiated
- defines basic variables and interface for all classes which can be partner in an interaction
- defines list of exposed quantities

System classes

The abstract class `system_t`:

```
type, extends(interaction_partner_t), abstract :: system_t

private
  class(propagator_t), pointer, public :: prop => null()

  integer         :: accumulated_loop_ticks
  integer, public :: interaction_timing  !< parameter to determine if interactions

  type(integer_list_t),     public :: supported_interactions
  type(interaction_list_t), public :: interactions !< List with all the interactions of this system

  type(mpi_grp_t), public :: grp  !< mpi group for this system
contains
  ! both deferred as actually defined methods
  ! ...
end type system_t
```

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type, extends(interaction_partner_t), abstract :: system_t

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  type(mpi_grp_t), public :: grp  !< mpi group for this system
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  ! ...
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```

- abstract class: cannot be instantiated
- inherits all from `interaction_partner_t`

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  integer, public :: interaction_timing  !< parameter to determine if interactions

  type(integer_list_t),     public :: supported_interactions
  type(interaction_list_t), public :: interactions !< List with all the interactions of this system

  type(mpi_grp_t), public :: grp  !< mpi group for this system
contains
  ! both deferred as actually defined methods
  ! ...
end type system_t
```

- abstract class: cannot be instantiated
- inherits all from `interaction_partner_t`
- defines basic variables and methods for all systems

System classes

The abstract class `system_t`:

```
type, extends(interaction_partner_t), abstract :: system_t

private
  class(propagator_t), pointer, public :: prop => null()

  integer         :: accumulated_loop_ticks
  integer, public :: interaction_timing  !< parameter to determine if interactions

  type(integer_list_t),     public :: supported_interactions
  type(interaction_list_t), public :: interactions !< List with all the interactions of this system

  type(mpi_grp_t), public :: grp  !< mpi group for this system
contains
  ! both deferred as actually defined methods
  ! ...
end type system_t
```

- abstract class: cannot be instantiated
- inherits all from `interaction_partner_t`
- defines basic variables and methods for all systems
- implements methods which are common to all systems

System classes

The abstract class `system_t`:

```
type, extends(interaction_partner_t), abstract :: system_t

private
  class(propagator_t), pointer, public :: prop => null()

  integer         :: accumulated_loop_ticks
  integer, public :: interaction_timing  !< parameter to determine if interactions

  type(integer_list_t),     public :: supported_interactions
  type(interaction_list_t), public :: interactions !< List with all the interactions of this system

  type(mpi_grp_t), public :: grp  !< mpi group for this system
contains
  ! both deferred as actually defined methods
  ! ...
end type system_t
```

- abstract class: cannot be instantiated
- inherits all from `interaction_partner_t`
- defines basic variables and methods for all systems
- implements methods which are common to all systems
- defines deferred methods which are common to all systems, but depend on specifics

System classes

The system_t methods:

```
procedure :: dt_operation =>  system_dt_operation
procedure :: reset_clocks => system_reset_clocks
procedure :: update_exposed_quantities => system_update_exposed_quantities
procedure :: init_propagator => system_init_propagator
procedure :: init_all_interactions => system_init_all_interactions
procedure :: init_parallelization => system_init_parallelization
procedure :: update_interactions => system_update_interactions
procedure :: update_interactions_start => system_update_interactions_start
procedure :: update_interactions_finish => system_update_interactions_finish
procedure :: propagation_start => system_propagation_start
procedure :: propagation_finish => system_propagation_finish
procedure :: has_reached_final_propagation_time => system_has_reached_final_propagation_time
procedure :: output_start => system_output_start
procedure :: output_write => system_output_write
procedure :: output_finish => system_output_finish
procedure :: process_is_slave => system_process_is_slave
procedure :: exec_end_of_timestep_tasks => system_exec_end_of_timestep_tasks

procedure(system_init_interaction),          deferred :: init_interaction
procedure(system_initial_conditions),        deferred :: initial_conditions
procedure(system_do_td_op),                  deferred :: do_td_operation
procedure(system_iteration_info),            deferred :: iteration_info
procedure(system_is_tolerance_reached),      deferred :: is_tolerance_reached
procedure(system_update_quantity),           deferred :: update_quantity
```

System classes

Child classes add more features to the parent class.

- deferred functions can be implemented
- functions of parent can be overridden

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Child classes add more features to the parent class.

- deferred functions can be implemented
- functions of parent can be overridden

Performing a algorithmic step: `dt_operation()`

- perform general tasks
- call `do_td_op()` of child class.

Classicle particles

`classical_particles_t`

- any number of classical particles
- described by array of 3-d vector for coordinates

Classicle particles

`classical_particles_t`

- any number of classical particles
- described by array of 3-d vector for coordinates

`classical_particle_t`

- specialized to one particle

Classicle particles

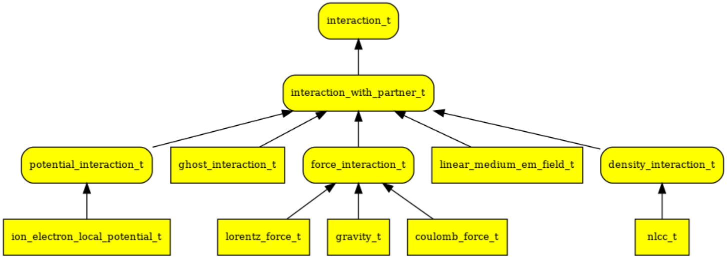
```
type, extends(system_t), abstract :: classical_particles_t

  private
  integer, public :: np                             !< Number of particles in the system
  FLOAT, allocatable, public :: mass(:)             !< Mass of the particles
  FLOAT, allocatable, public :: pos(:,:)            !< Position of the particles
  FLOAT, allocatable, public :: vel(:,:)            !< Velocity of the particles
  FLOAT, allocatable, public :: tot_force(:,:) !< Total force acting on each particle
  logical, allocatable, public :: fixed(:)          !< True if a giving particle is to be kept fixed during a
                                                    !< propagation. The default is to let the particles move.

  !> The following variables are work arrays used by the different propagators:
  FLOAT, allocatable :: acc(:,:)               !< Acceleration of the particles
  FLOAT, allocatable :: prev_acc(:,:,:)        !< A storage of the prior times.
  FLOAT, allocatable :: save_pos(:,:)          !< A storage for the SCF loops
  FLOAT, allocatable :: save_vel(:,:)          !< A storage for the SCF loops
  FLOAT, allocatable :: prev_tot_force(:,:) !< Used for the SCF convergence criterium
  FLOAT, allocatable :: prev_pos(:,:,:)        !< Used for extrapolation
  FLOAT, allocatable :: prev_vel(:,:,:)        !< Used for extrapolation
  FLOAT, allocatable :: hamiltonian_elements(:,:)

contains

  procedure :: do_td_operation => classical_particles_do_td
  procedure :: is_tolerance_reached => classical_particles_is_tolerance_reached
  procedure :: copy_quantities_to_interaction => classical_particles_copy_quantities_to_interaction
  procedure :: update_interactions_start => classical_particles_update_interactions_start
  procedure :: update_interactions_finish => classical_particles_update_interactions_finish

end type classical_particles_t
```

Classicle particles

```
type, extends(classical_particles_t) :: classical_particle_t

  type(c_ptr) :: output_handle

contains

  procedure :: init_interaction => classical_particle_init_interaction
  procedure :: initial_conditions => classical_particle_initial_conditions
  procedure :: iteration_info => classical_particle_iteration_info
  procedure :: output_start => classical_particle_output_start
  procedure :: output_write => classical_particle_output_write
  procedure :: output_finish => classical_particle_output_finish
  procedure :: update_quantity => classical_particle_update_quantity
  procedure :: update_exposed_quantity => classical_particle_update_exposed_quantity
  procedure :: init_interaction_as_partner => classical_particle_init_interaction_as_partner
  procedure :: copy_quantities_to_interaction => classical_particle_copy_quantities_to_interaction
  final :: classical_particle_finalize

end type classical_particle_t
```

Interaction classes

Currently implemented interaction classes:



- `potential_interaction_t`: acting on electrons (in development)
- `force_interaction_t`: acting on classical particles
- `linear_medium_em_t`: acting on Maxwell fields

Interaction classes

The abstract class `interaction_t`:

```
type, abstract :: interaction_t

  private

  !> The interaction requires access to some quantities from a system to be evaluated.

  integer,              public :: n_system_quantities  !< Number of quantities needed from the system
  integer, allocatable, public :: system_quantities(:) !< Identifiers of the quantities needed from the system
  type(clock_t), public :: clock !< Clock storing the time at which the interaction was last updated.
  character(len=:), public, allocatable :: label

contains

  procedure(interaction_update),    deferred :: update
  procedure(interaction_calculate), deferred :: calculate

end type interaction_t
```

Interaction classes

The abstract class `interaction_with_partner_t`:

```
!> Some interactions involve two systems. In this case the interaction is a
!! unidirectional relationship between those two systems. One of the systems
!! owns the interaction and feels its effects. The other system is referred to
!! as the interaction partner.

type, extends(interaction_t), abstract :: interaction_with_partner_t

  private

  class(interaction_partner_t), public, pointer :: partner
  integer,              public :: n_partner_quantities  !< Number of quantities needed from the partner
  integer, allocatable, public :: partner_quantities(:) !< Identifiers of the quantities needed
                                                        !< from the partner

contains

  procedure :: update => interaction_with_partner_update

end type interaction_with_partner_t
```

Interaction classes

The abstract class `force_interaction_t`:

```
type, extends(interaction_with_partner_t), abstract :: force_interaction_t

  integer :: dim = 0       !< spatial dimensions
  integer :: system_np = 0 !< number of particles in the system that the forces are acting on

  FLOAT, allocatable, public :: force(:,:)
end type force_interaction_t
```

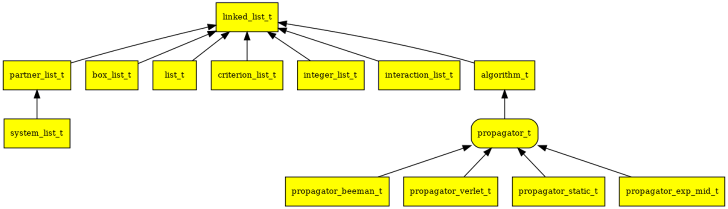
Interaction classes

The class `gravity_t`:

```
!> Gravity interaction between two systems of particles. This should be used
!! for testing purposes only. Note that this interaction assumes all
!! quantities are in S.I. units instead of atomic units.
type, extends(force_interaction_t) :: gravity_t
  private
  FLOAT, pointer :: system_mass(:) !< pointer to array storing the masses of the particles
  FLOAT, pointer :: system_pos(:,:) !< pointer to array storing the positions of the particles

  integer, public :: partner_np = 0 !< number of particles in the partner system
  FLOAT, allocatable, public :: partner_mass(:)  !< array storing a copy of the masses of the
                                                 !< partner particles
  FLOAT, allocatable, public :: partner_pos(:,:) !< array storing a copy of the positions of the
                                                 !< partner particles

contains
  procedure :: init => gravity_init
  procedure :: calculate => gravity_calculate
  final :: gravity_finalize
end type gravity_t
```

Propagator implementation

Class hierarchy of propagators:



As propagators are derived from linked lists and algorithms, one can directly use their respective methods.

Propagator implementation

Defining a propagator:

```
function propagator_verlet_constructor(dt) result(this)
  FLOAT,                      intent(in) :: dt
  type(propagator_verlet_t), pointer    :: this

  PUSH_SUB(propagator_verlet_constructor)

  SAFE_ALLOCATE(this)

  this%start_step = OP_VERLET_START
  this%final_step = OP_VERLET_FINISH

  call this%add_operation(OP_VERLET_UPDATE_POS)
  call this%add_operation(OP_UPDATE_INTERACTIONS)
  call this%add_operation(OP_VERLET_COMPUTE_ACC)
  call this%add_operation(OP_VERLET_COMPUTE_VEL)
  call this%add_operation(OP_FINISHED)

  ! Verlet has only one algorithmic step
  this%algo_steps = 1

  this%dt = dt

  POP_SUB(propagator_verlet_constructor)
end function propagator_verlet_constructor
```

Propagator implementation

Defining a propagator:

```
! Specific verlet propagation operations identifiers
character(len=30), public, parameter ::      &
  VERLET_START       = 'VERLET_START',       &
  VERLET_FINISH      = 'VERLET_FINISH',      &
  VERLET_UPDATE_POS  = 'VERLET_UPDATE_POS',  &
  VERLET_COMPUTE_ACC = 'VERLET_COMPUTE_ACC', &
  VERLET_COMPUTE_VEL = 'VERLET_COMPUTE_VEL'

! Specific verlet propagation operations
type(algorithmic_operation_t), public, parameter :: &
  OP_VERLET_START       = algorithmic_operation_t(VERLET_START,       'Starting Verlet propagation'),
  OP_VERLET_FINISH      = algorithmic_operation_t(VERLET_FINISH,      'Finishing Verlet propagation'),
  OP_VERLET_UPDATE_POS  = algorithmic_operation_t(VERLET_UPDATE_POS,  'Propagation step - Updating positions'),
  OP_VERLET_COMPUTE_ACC = algorithmic_operation_t(VERLET_COMPUTE_ACC, 'Propagation step - Computing acceleratio
  OP_VERLET_COMPUTE_VEL = algorithmic_operation_t(VERLET_COMPUTE_VEL, 'Propagation step - Computing velocity')
```

These are defined as module variables.

Propagator implementation

Implementing the steps: `system_t%do_td_operation()`

- Actual tasks depend on the specific system.
- the specific function is the same for all implemented algorithms
- $\Rightarrow$ implement operations for all implemented propagators

Propagator implementation

Implementing the steps: `system_t%do_td_operation()`

```
subroutine classical_particles_do_td(this, operation)
  class(classical_particles_t),    intent(inout) :: this
  class(algorithmic_operation_t),  intent(in)    :: operation
  ...
  select case (operation%id)
  case (SKIP)
    ! Do nothing
  case (STORE_CURRENT_STATUS)
    this%save_pos(:, 1:this%np) = this%pos(:, 1:this%np)
    this%save_vel(:, 1:this%np) = this%vel(:, 1:this%np)

  case (VERLET_FINISH)
    ...
  case (BEEMAN_FINISH)
    ...
  case (VERLET_UPDATE_POS)
    this%pos(:, 1:this%np) = this%pos(:, 1:this%np) + this%prop%dt * this%vel(:, 1:this%np) &
      + M_HALF * this%prop%dt**2 * this%acc(:, 1:this%np)
    this%quantities(POSITION)%clock = this%quantities(POSITION)%clock + CLOCK_TICK

  ...
```