PSyclone LFRic distributed memory support

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ESIWACE2 training course on Domain-specific Languages in Weather and Climate, 23rd-27th November 2020

Overview

- 90 minute session
- Hands on part 1 : 15 minutes
  - Going parallel
- Introduction to distributed memory : 30 minutes
- Hands on part 2 : 45 minutes
  - 3 parts
    - Annexed dofs
    - Asynchronous comms
    - Reductions
- Any issues/questions on the slack channel

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Hands-on : Let's go parallel

- 15 minutes
- `cd <psyclone_home>/tutorial/practicals/LFRic/distributed_memory/1_distributed_memory`
- No compilation, just code generation
- Follow the `README.md` in the directory
  - A browser will display `README.md` files nicely
  - `https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/distributed_memory/1_distributed_memory`
- Any issues/questions on slack
  - Use the psyclone channel
  - Please use threads for replies

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Going parallel: Summary

- Example code extracted from LFRic – most computationally costly part of the dynamical core
- The same algorithm and kernel code written by the scientist is used to run serially or in parallel
  - Single-source science code
  - Science code is not concerned with parallel implementation
- For a user, generating serial or distributed memory parallel code is controlled by a single PSyclone command-line argument

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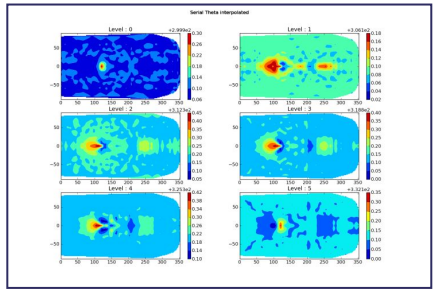
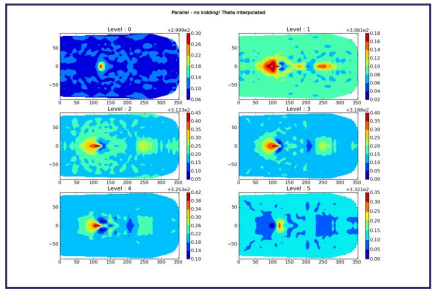
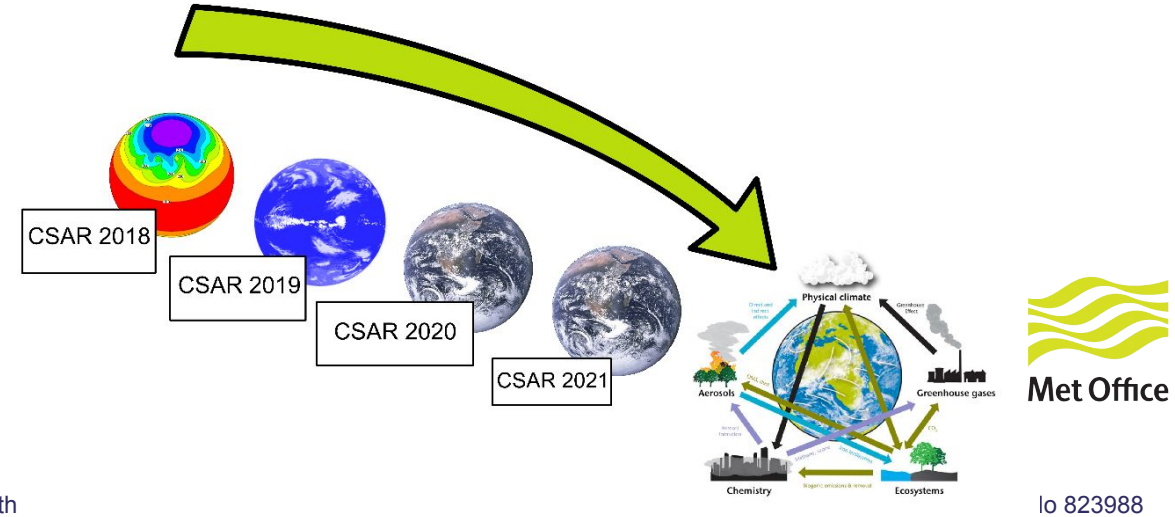
Going parallel: In practice





- PSyclone integrated into LFRic build system in September 2015 - serial
- LFRic went parallel (MPI + OpenMP) in March 2016
  - Switch was essentially immediate (but took 1 week in practice due to simple PSyclone OpenMP bug for reductions)
  - No change to science code from serial to parallel
- Science development has continued since then (including adding Physics)



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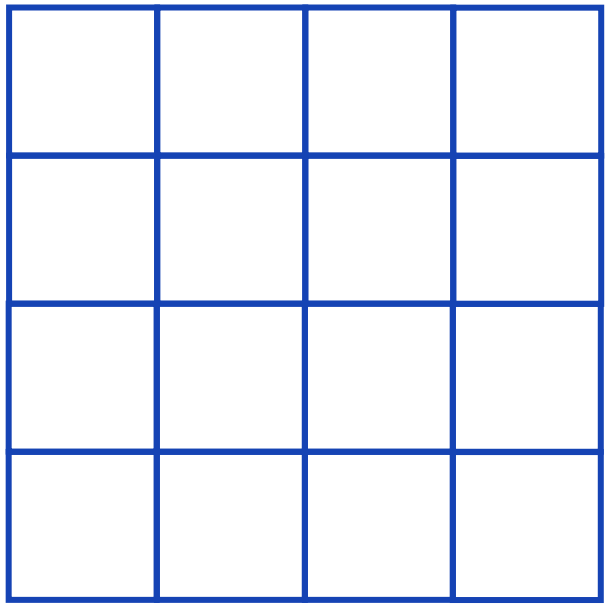
Cells/Elements



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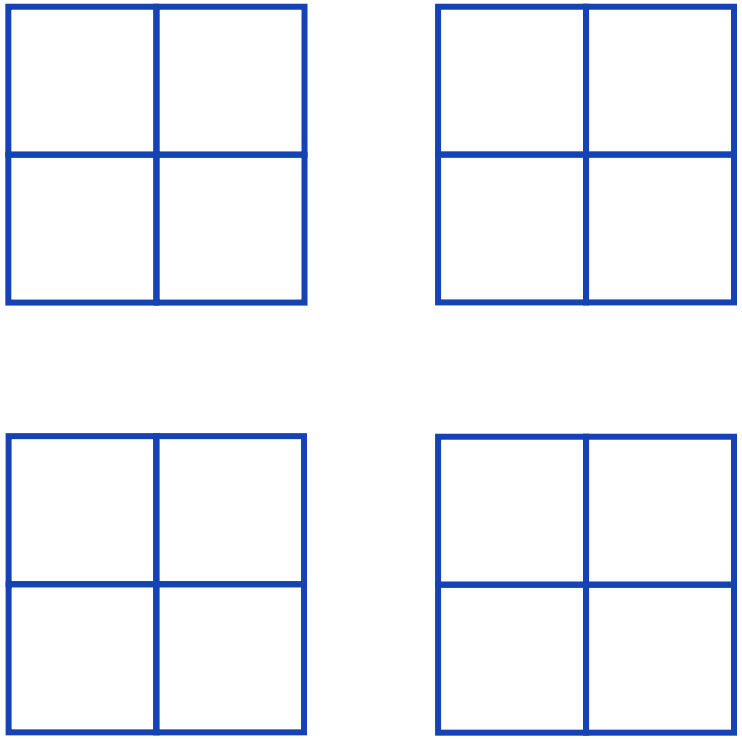
Partitioned Cells/Elements



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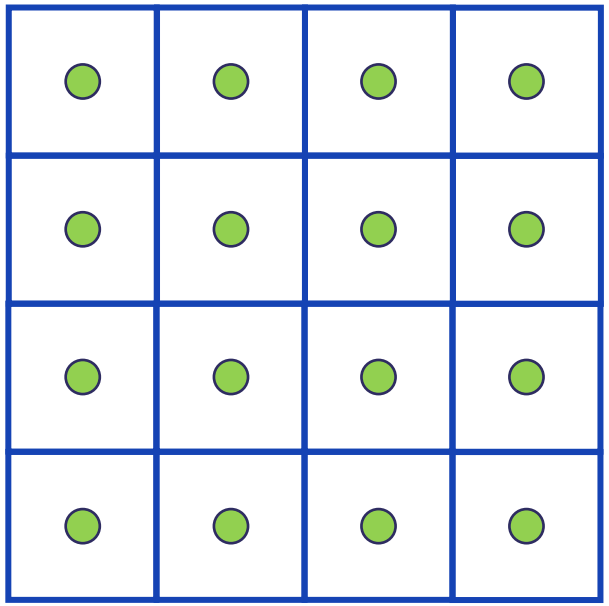
DOFs on discontinuous function space



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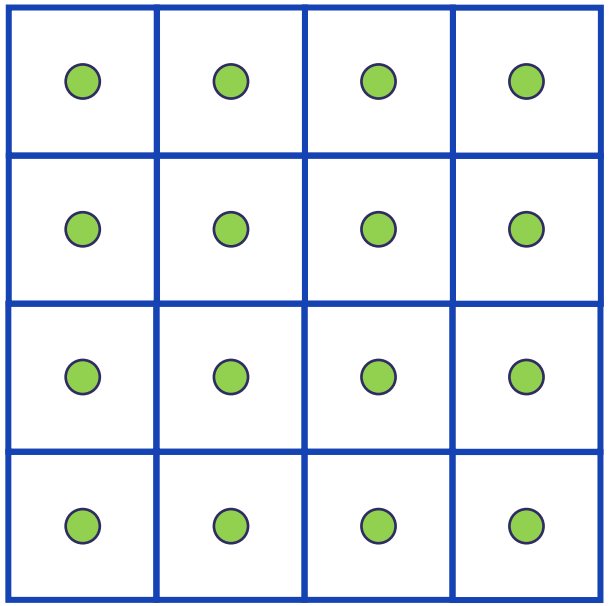
Iterating over discontinuous DOFs

Iterate over dofs

```
DO i=1,ndofs
    ! builtin code
```



Accesses

```
read
write
readwrite
```

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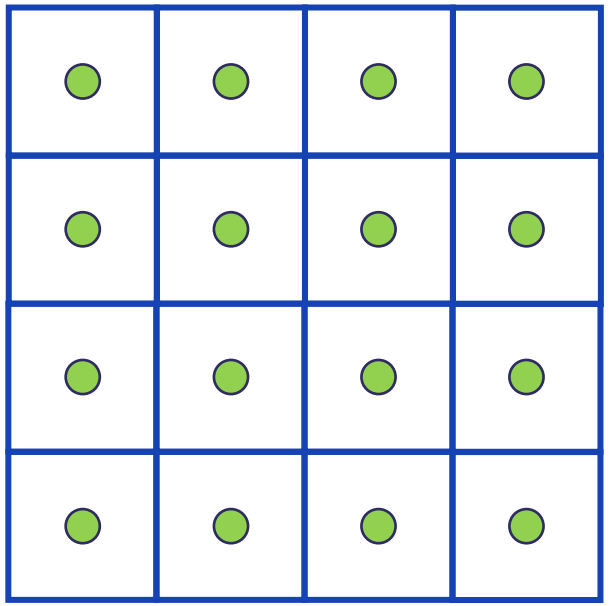
Iterating over cells with discontinuous DOFs

Iterate over cells

```
DO i=1,ncells
    call kern(…)
```



Accesses

```
read
write
readwrite
```

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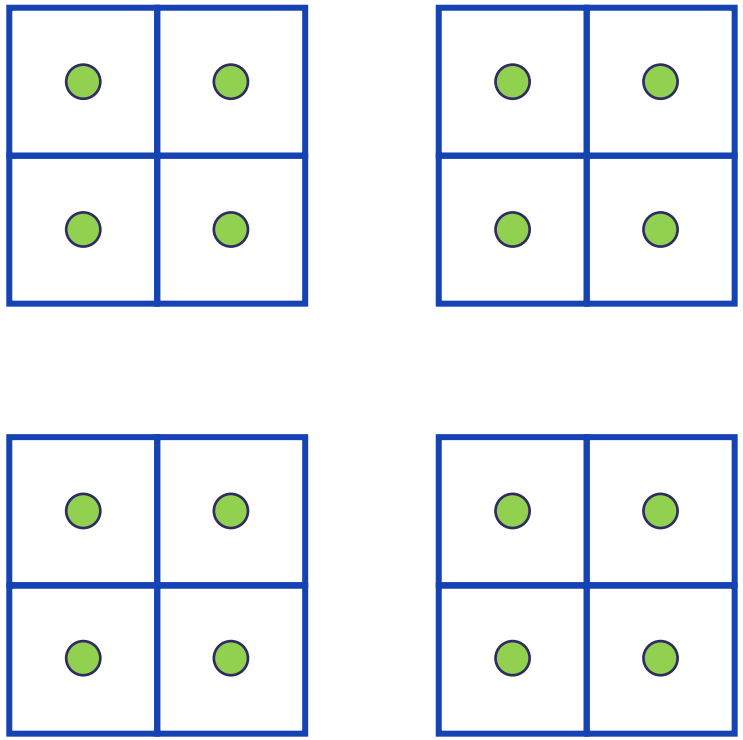
Partitioned discontinuous DOFs

Iterate over dofs

```
DO i=1,ndofs
    ! builtin code
```



Iterate over cells

```
DO i=1,ncells
    call kern(…)
```

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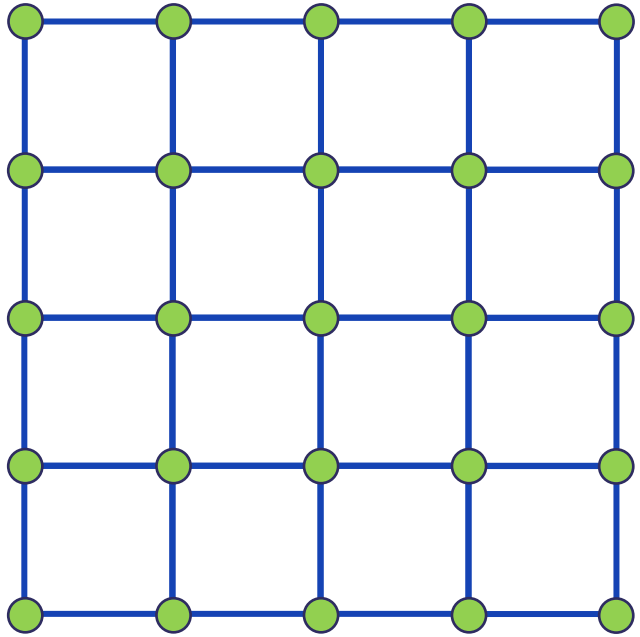
DOFs on a continuous function space



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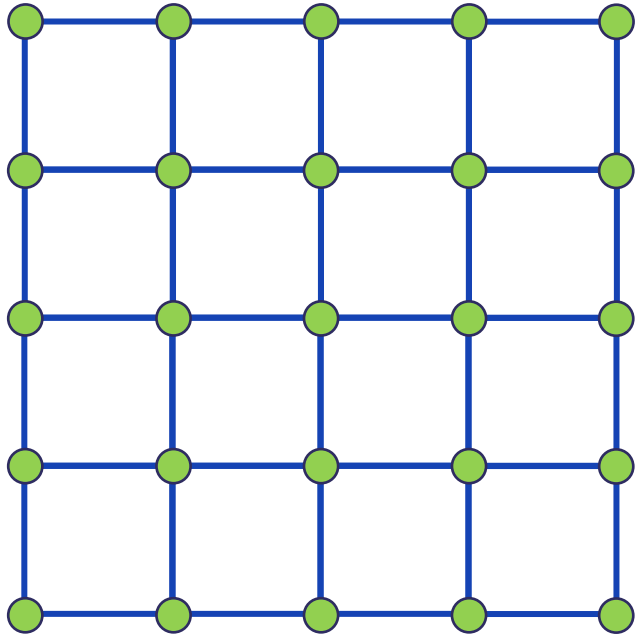
Iterating over continuous DOFs

Iterate over dofs

```
DO i=1,ndofs
    ! builtin code
```



Accesses

```
read
write
readwrite
```

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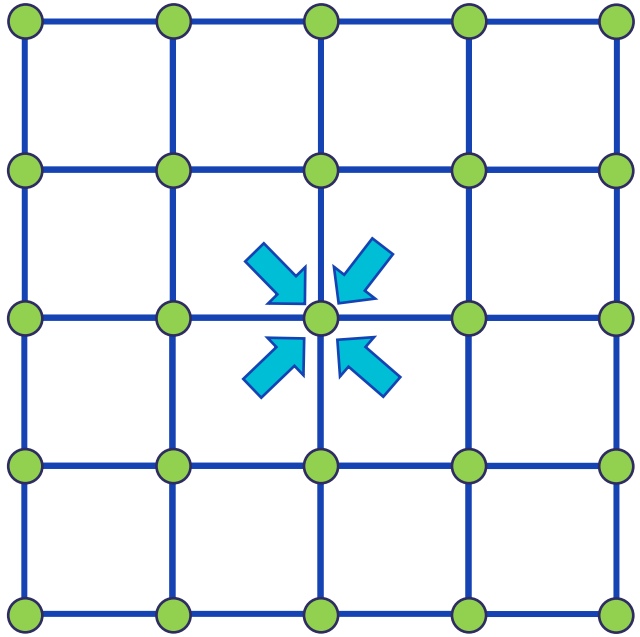
Iterating over cells with continuous DOFs

Iterate over cells

```
DO i=1,ncells
    call kern(…)
```



Accesses

```
read
inc
```

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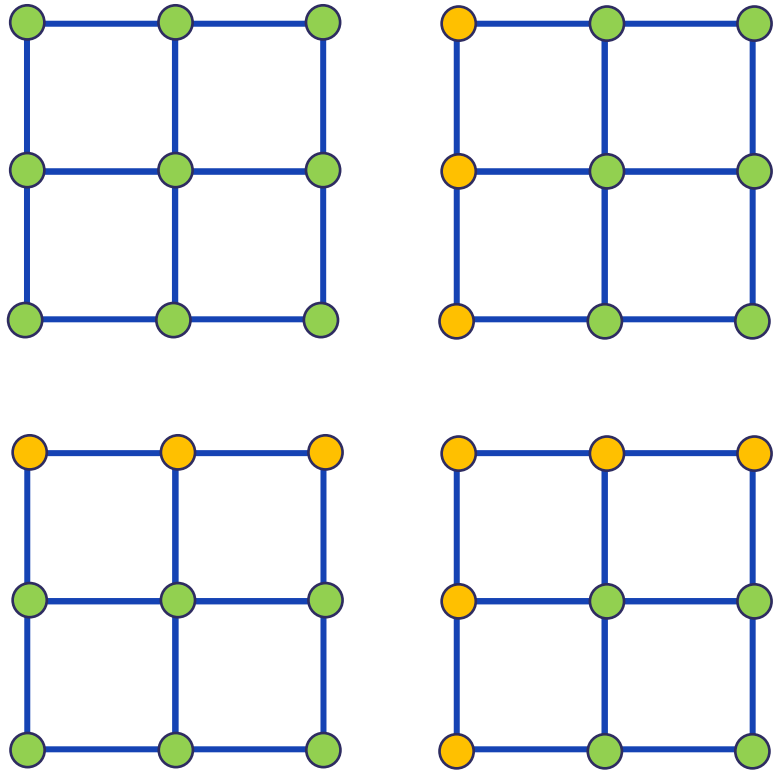
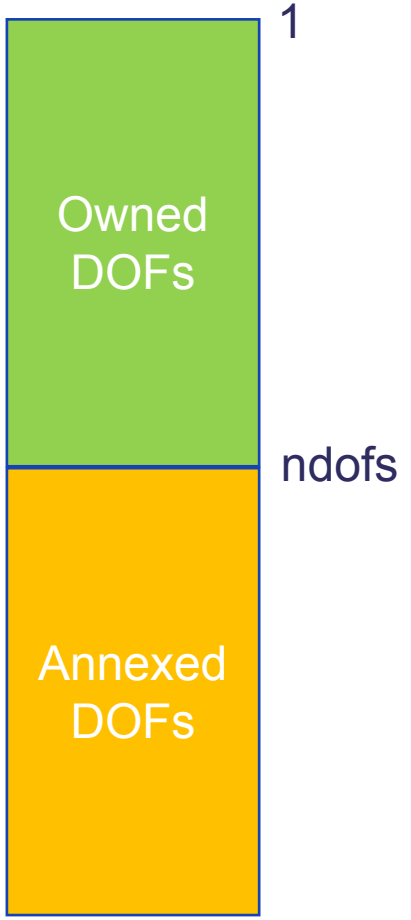
Partitioned continuous DOFs

Iterate over dofs

```
DO i=1,ndofs
    ! builtin code
```



DOFs Numbering scheme



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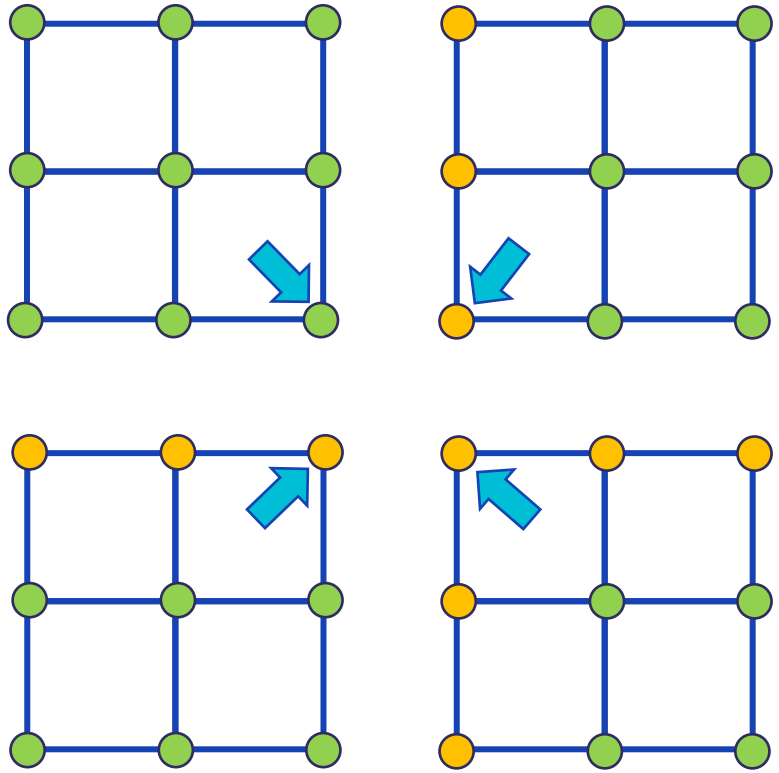
Partial sums

Iterate over cells

```
DO i=1,ncells
   call kern(…)
```



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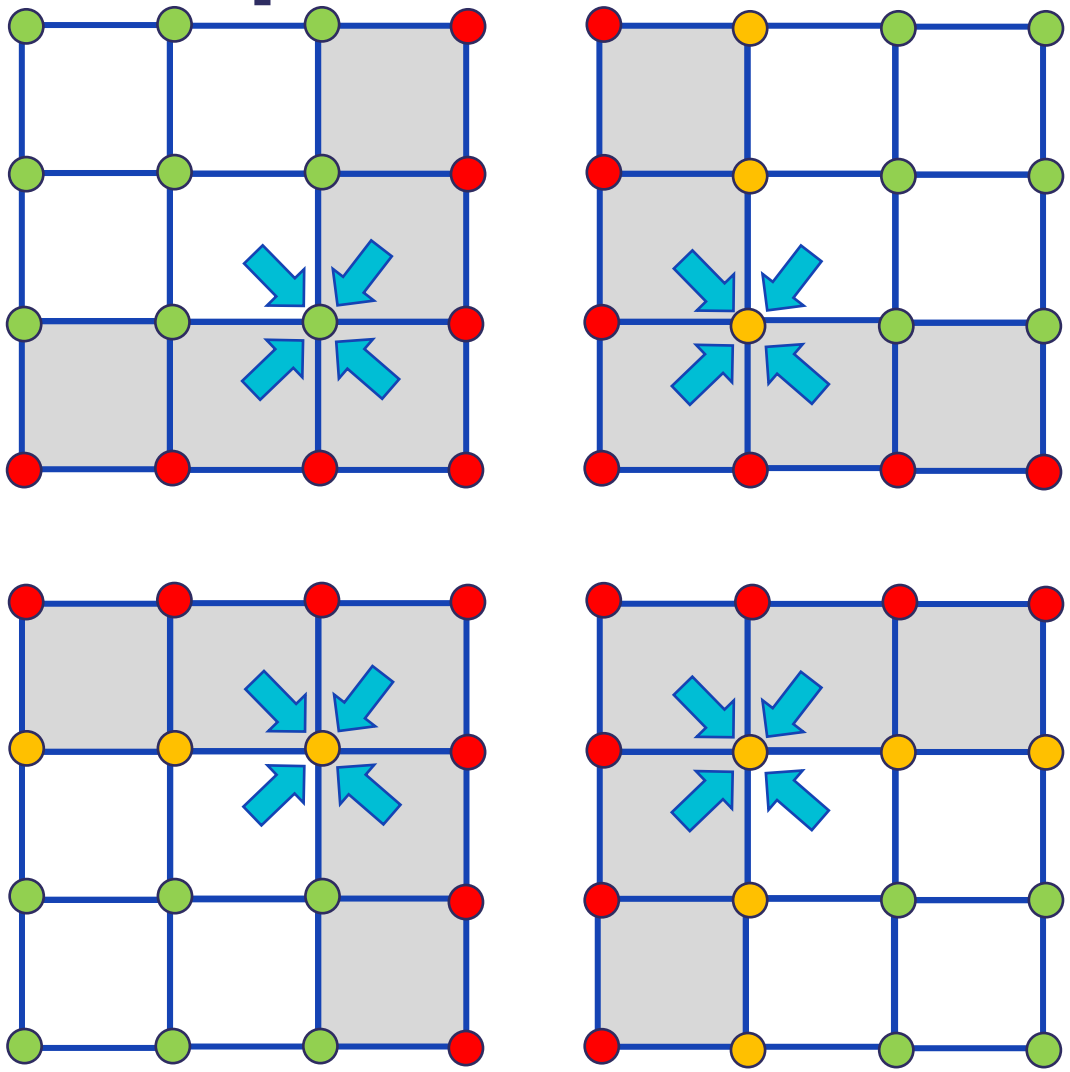
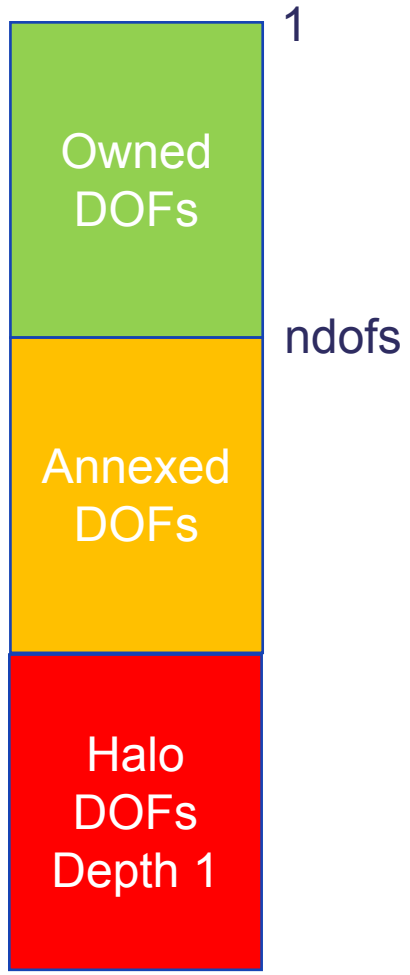
Redundant computation

Iterate over cells

```
DO i=1,cell_halo(1)
    call kern()
```



DOFs Numbering scheme



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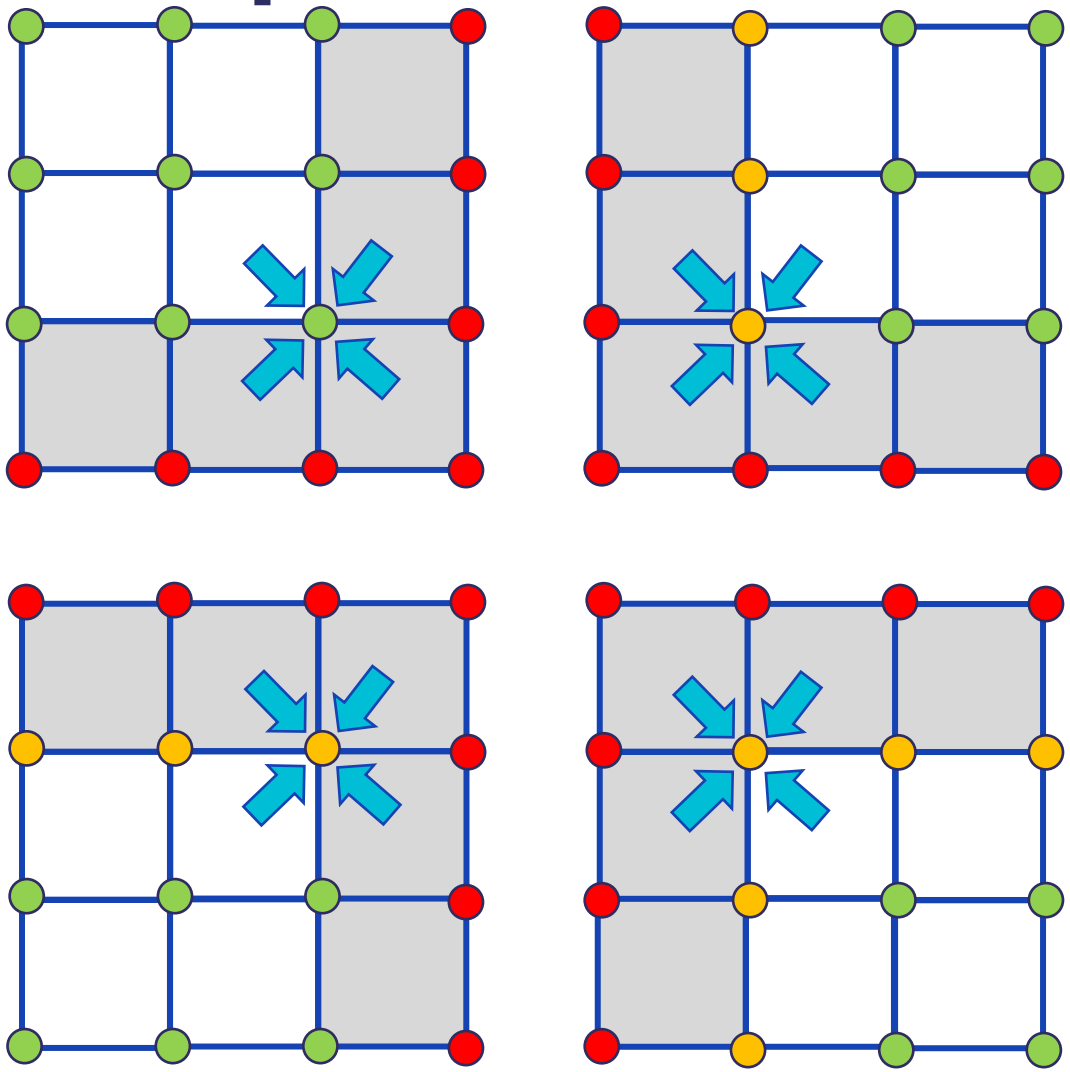
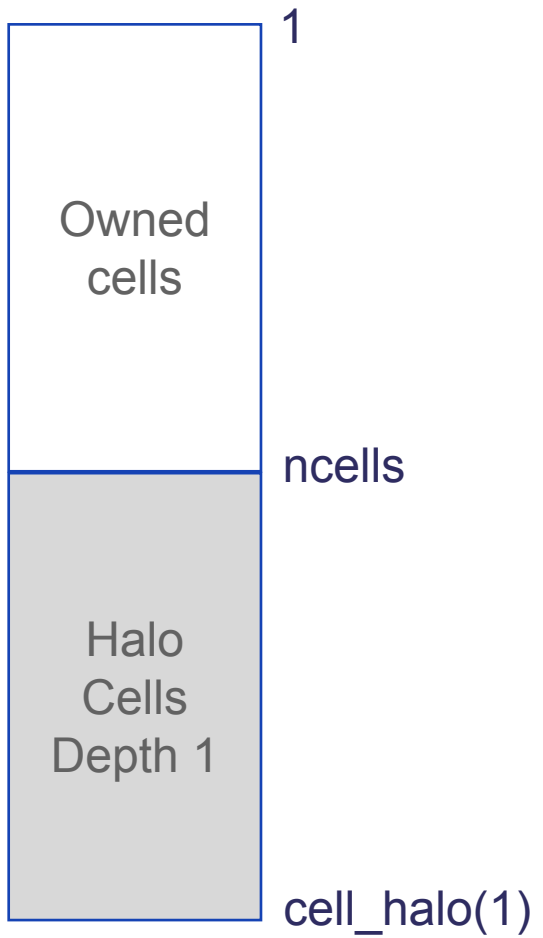
Redundant computation

Iterate over cells

```
DO i=1,cell_halo(1)
    call kern()
```



Cells Numbering scheme



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PSyIR view

```
InvokeSchedule[invoke='invoke_0', dm=True]
    0: Loop[type='dofs', field_space='any_space_1', it_space='dof', upper_bound='ndofs']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: BuiltIn setval_c(grad_p,0.0_r_def)
    1: HaloExchange[field='grad_p', type='region', depth=1, check_dirty=False]
    2: HaloExchange[field='p', type='region', depth=1, check_dirty=True]
    3: HaloExchange[field='div_star', type='region', depth=1, check_dirty=True]
    4: HaloExchange[field='hb_inv', type='region', depth=1, check_dirty=True]
    5: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern scaled_matrix_vector_code(grad_p,p,div_star,hb_inv) [module_inline=False]
    6: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern enforce_bc_code(grad_p) [module_inline=False]
    7: HaloExchange[field='mt_lumped_inv', type='region', depth=1, check_dirty=True]
    8: Loop[type='', field_space='w3', it_space='cell_column', upper_bound='ncells']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern apply_variable_hx_code(hp,grad_p,mt_lumped_inv,p,compound_div,p3theta,ptheta2,m3_exner_star,tau_t,timeste
p_term) [module_inline=False]
```

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Halo exchange logic

```
InvokeSchedule[invoke='invoke_0', dm=True]
    0: Loop[type='dofs', field_space='any_space_1', it_space='dof', upper_bound='ndofs']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: BuiltIn setval_c(grad_p,0.0_r_def)
    1: HaloExchange[field='grad_p', type='region', depth=1, check_dirty=False]
    2: HaloExchange[field='p', type='region', depth=1, check_dirty=True]
    3: HaloExchange[field='div_star', type='region', depth=1, check_dirty=True]
    4: HaloExchange[field='hb_inv', type='region', depth=1, check_dirty=True]
    5: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern scaled_matrix_vector_code(grad_p,p,div
    6: Loop[type='', field_space='any_space_1', it_space='cell_
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFI
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFI
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern enforce_bc_code(grad_p) [module_inline
    7: HaloExchange[field='mt_lumped_inv', type='region', depth
    8: Loop[type='', field_space='w3', it_space='cell_column',
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFI
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFI
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern apply_variable_hx_code(hp,grad_p,mt_lu
p_term) [module_inline=False]
```

Loop 1
Writes to `grad_p`
`1` to `ndofs`
Makes `grad_p` halo dofs “dirty”
Makes `grad_p` annexed dofs “dirty”
No reads
No halo exchange needed

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Halo exchange logic

```
InvokeSchedule[invoke='invoke_0', dm=True]
    0: Loop[type='dofs', field_space='any_space_1', it_space='dof', upper_bound='ndofs']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: BuiltIn setval_c(grad_p,0.0_r_def)
    1: HaloExchange[field='grad_p', type='region', depth=1, check_dirty=False]
    2: HaloExchange[field='p', type='region', depth=1, check_dirty=True]
    3: HaloExchange[field='div_star', type='region', depth=1, check_dirty=True]
    4: HaloExchange[field='hb_inv', type='region', depth=1, check_dirty=True]
    5: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern scaled_matrix_vector_code(grad_
    6: Loop[type='', field_space='any_space_1', it_space
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern enforce_bc_code(grad_p) [module
    7: HaloExchange[field='mt_lumped_inv', type='region'
    8: Loop[type='', field_space='w3', it_space='cell_co
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER,
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern apply_variable_hx_code(hp,grad_
p_term) [module_inline=False]
```

Loop 2
modifies `grad_p` [continuous?]
`1` to `cell_halo(1)`
Makes `grad_p` halo depth 1 dofs “dirty”
Makes `grad_p` annexed dofs “clean”
Needs `grad_p` annexed dofs
Loop 1 makes them “dirty”
Halo exchange needed

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Halo exchange logic

```
InvokeSchedule[invoke='invoke_0', dm=True]
    0: Loop[type='dofs', field_space='any_space_1', it_space='dof', upper_bound='ndofs']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: BuiltIn setval_c(grad_p,0.0_r_def)
    1: HaloExchange[field='grad_p', type='region', depth=1, check_dirty=False]
    2: HaloExchange[field='p', type='region', depth=1, check_dirty=True]
    3: HaloExchange[field='div_star', type='region', depth=1, check_dirty=True]
    4: HaloExchange[field='hb_inv', type='region', depth=1, check_dirty=True]
    5: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern scaled_matrix_vector_code(grad_p,p,div_star,hb_inv) [module_inline=False]
    6: Loop[type='', field_space='any_space_1', it_space='cell_column', upper_bound='cell_halo(1)']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFIN
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern enforce_bc_code(grad_p) [module_inline=
    7: HaloExchange[field='mt_lumped_inv', type='region', depth=
    8: Loop[type='', field_space='w3', it_space='cell_column', u
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFIN
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFIN
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern apply_variable_hx_code(hp,grad_p,mt_lum
p_term) [module_inline=False]
```

Loop 2
reads `p`, `div_star`, `hb_inv`
`1` to `cell_halo(1)`
Halo exchange needed if halos are "dirty": runtime check

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Runtime dirty flags

```
      DO df=1,grad_p_proxy%vspace%get_last_dof_owned()
        grad_p_proxy%data(df) = 0.0_r_def
      END DO
      !
      ! Set halos dirty/clean for fields modified in the above loop
      !
      CALL grad_p_proxy%set_dirty()
      !
      CALL grad_p_proxy%halo_exchange(depth=1)
      !
      IF (p_proxy%is_dirty(depth=1)) THEN
        CALL p_proxy%halo_exchange(depth=1)
      END IF
      !
      IF (div_star_proxy%is_dirty(depth=1)) THEN
        CALL div_star_proxy%halo_exchange(depth=1)
      END IF
      !
      IF (hb_inv_proxy%is_dirty(depth=1)) THEN
        CALL hb_inv_proxy%halo_exchange(depth=1)
      END IF
      !
      DO cell=1,mesh%get_last_halo_cell(1)
        !
        CALL scaled_matrix_vector_code(nlayers, grad_p_proxy%data, p_proxy%data, div_star_proxy%data, hb_inv_proxy%data, ndf_aspc1_gr
ad_p, undf_aspc1_grad_p, map_aspc1_grad_p(:,cell), ndf_aspc2_p, undf_aspc2_p, map_aspc2_p(:,cell), ndf_w3, undf_w3, map_w3(:,cell))
      END DO
      !
      ! Set halos dirty/clean for fields modified in the above loop
      !
      CALL grad_p_proxy%set_dirty()
```

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“Annexed dofs” optimisation

- LFRic either loops over cells or dofs
- If we iterate over cells, we always guarantee that the annexed dofs for a modified continuous field will be clean due to redundant computation
- If we always redundantly compute annexed dofs when we iterate over dofs there will be no additional halo exchanges required
- We have seen in example 1 that dirty annexed dofs may result in halo exchanges
- So …
- Redundantly compute “annexed dofs” for the whole code then we can assume that annexed dofs are always clean and potentially reduce the number of halo exchanges

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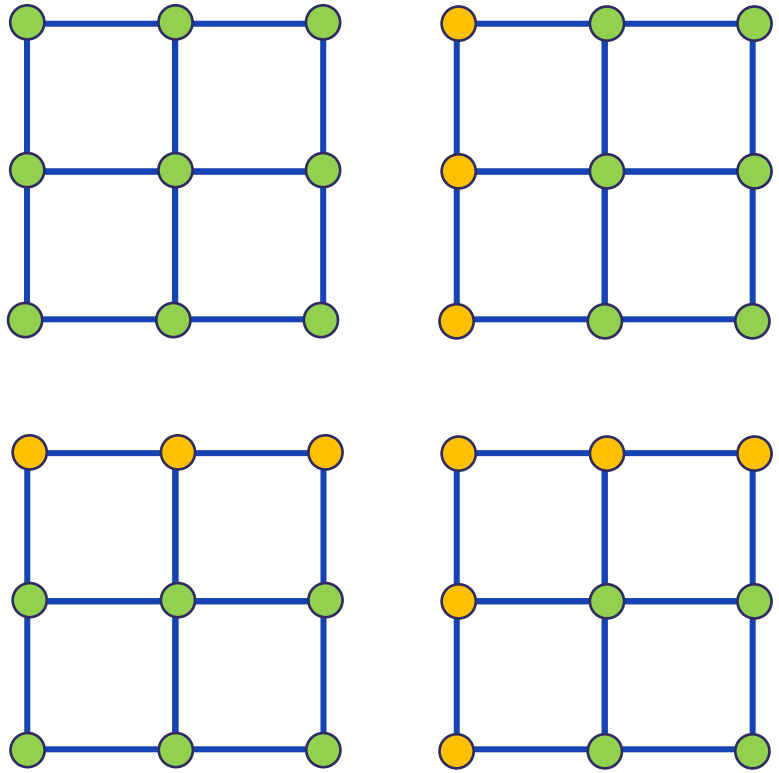
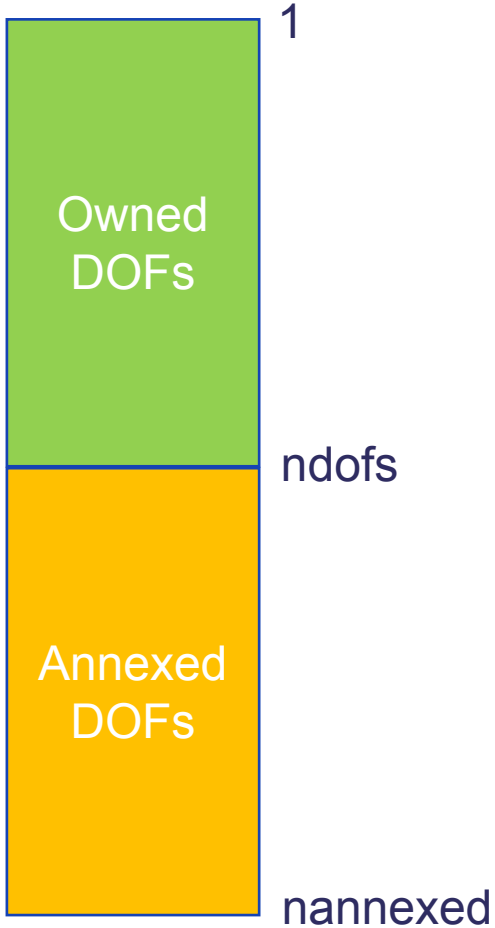
Partitioned continuous DOFs

Iterate over dofs

```
DO i=1,nannexed
    ! builtin code
```



DOFs Numbering scheme



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Annexed dofs: Halo exchange reduction

Number of halo exchanges	% reduction	Description
63,668		LFRic Fallow Deer release
63,000	1%	GH_INC : no halo exchange for increments
46,274	27%	ANNEXED : redundantly compute annexed dofs
19,892	69%	ANNEXED + GH_INC

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Overlapping communication with computation

- If you can't avoid a halo exchange then you could try to overlap it with computation
- PSyclone provides 2 transformations to help with this
  1. A transformation that changes the default synchronous halo exchange into an asynchronous halo exchange
  2. A transformation that moves PSyIR nodes which, in this case, can be used to make halo exchanges overlap with computation

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Supporting reductions

- LFRic and PSyclone support two types of communication pattern
  - nearest neighbour (stencil) communication patterns - halo exchanges
  - Reductions

```
do i = 1, n
  a = a + data(i)
end do
```

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What else?

- Now
  - Arbitrary depth redundant computation via a PSyclone transformation

- Future
  - Loop splitting (into internal computation and halo computation)
  - Communication aggregation
  - Eager (asynchronous) halo exchange protocol
  - Test working with partial sums and annexed dofs instead of redundant computation in the halo?
  - Non-MPI based comms?

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Hands on

- ~45 minutes
- `cd <psyclone_home>/tutorial/practicals/LFRic/distributed_memory`
- 3 parts `2_annexed_dofs, 3_overlapping_comms, 4_reductions`
- No compilation, just code generation
- Follow the `README.md` in the directories
  - A browser will display `README.md` files nicely
  - https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/distributed_memory
- Any issues/questions on slack
  - Use the psyclone channel
  - Please use threads for replies

Have fun!

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