Computing for Climate Modelling

Scott Wales, CLEX CMS

CLEX CMS | cws_help@nci.org.au

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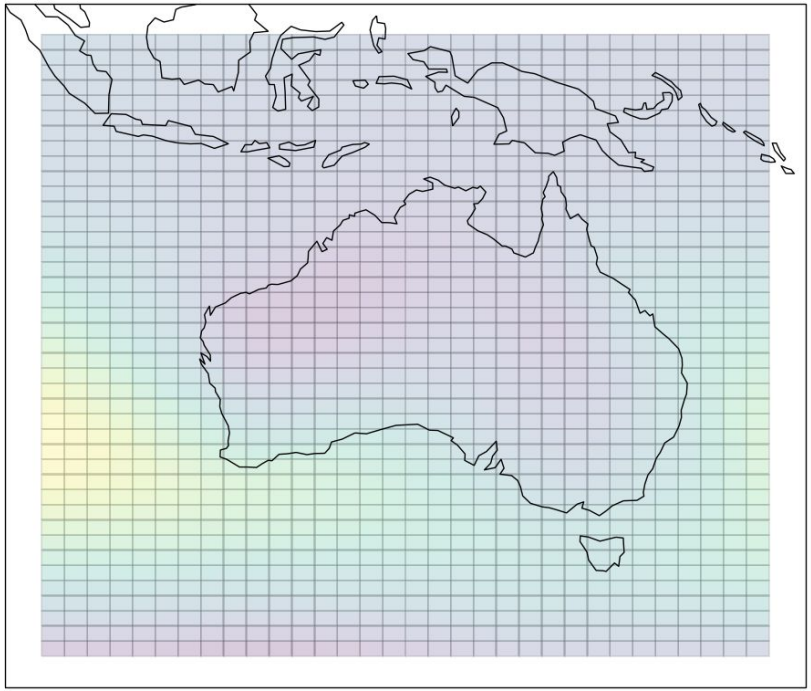
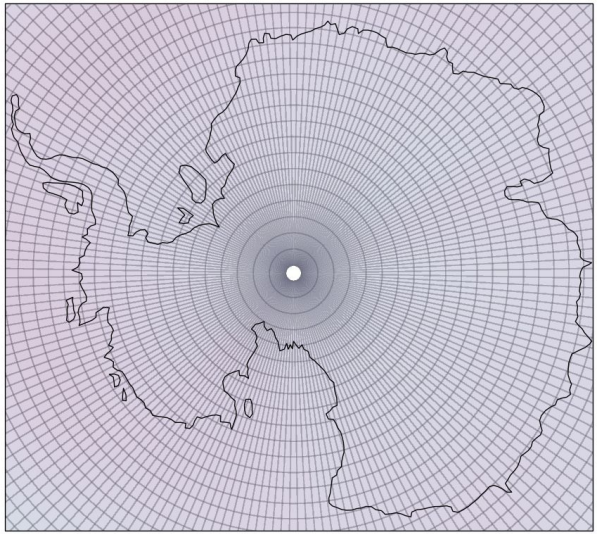
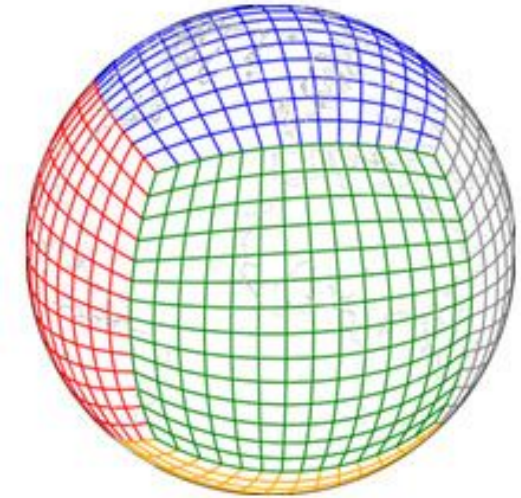
Discretisation





Alternate Grid Types

Cubed Sphere

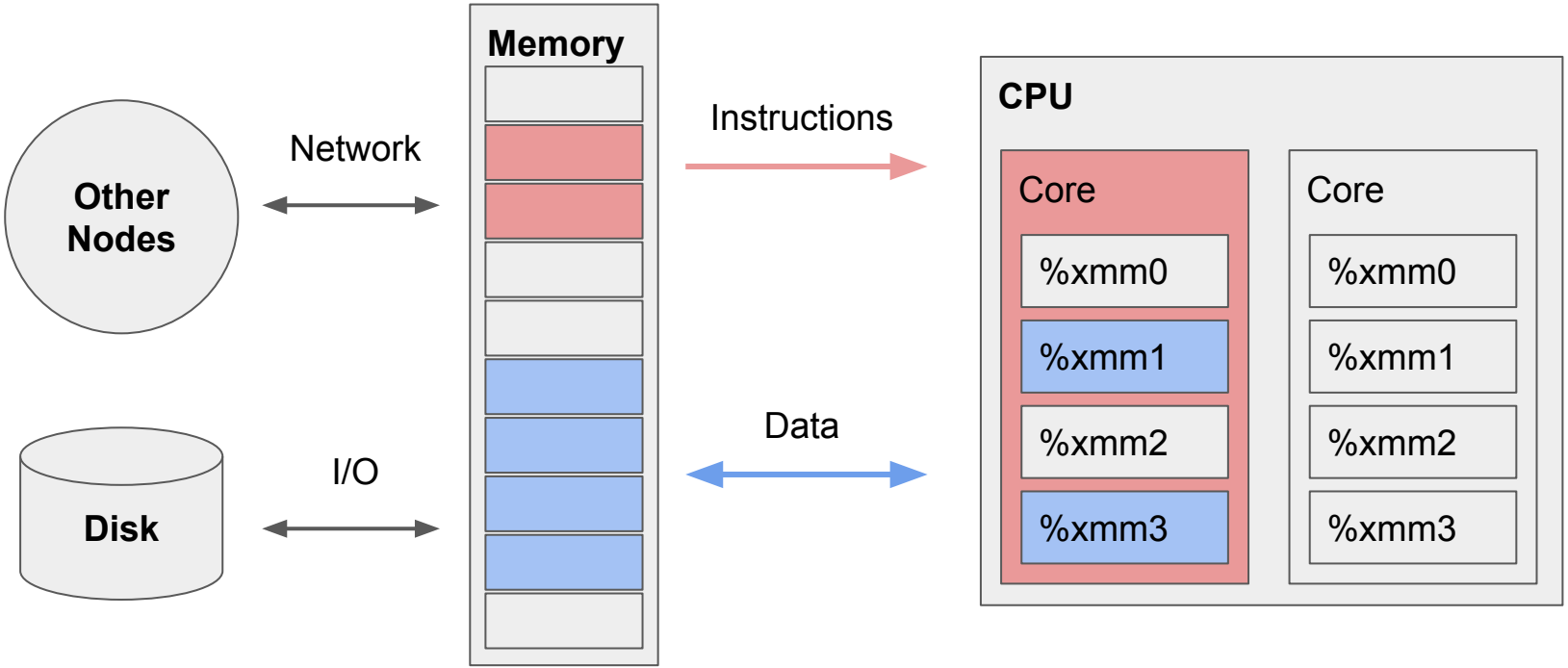


https://www.gfdl.noaa.gov/fv3/fv3-grids/

Voronoi Tessellation

https://mpas-dev.github.io/

Compute Node



Compiling

Fortran:

```
subroutine add(r, a, b)
    real, intent(in) :: a(4), b(4)
    real, intent(out) :: r(4)
    integer :: i

    do i=1,4
        r(i) = a(i) + b(i)
    end do
end subroutine
```

Assembly:

```
add_:
# parameter 1: %rdi
# parameter 2: %rsi
# parameter 3: %rdx
        movups    (%rsi), %xmm1          #5.5
        movups    (%rdx), %xmm0          #5.5
        addps     %xmm0, %xmm1           #5.5
        movups    %xmm1, (%rdi)          #5.5
        ret                              #6.1
```

Memory Layout

Model Field

1,1	1,2	1,3	1,4
2,1	2,2	2,3	2,4
3,1	3,2	3,3	3,4
4,1	4,2	4,3	4,4

Computer Memory

Parallelisation

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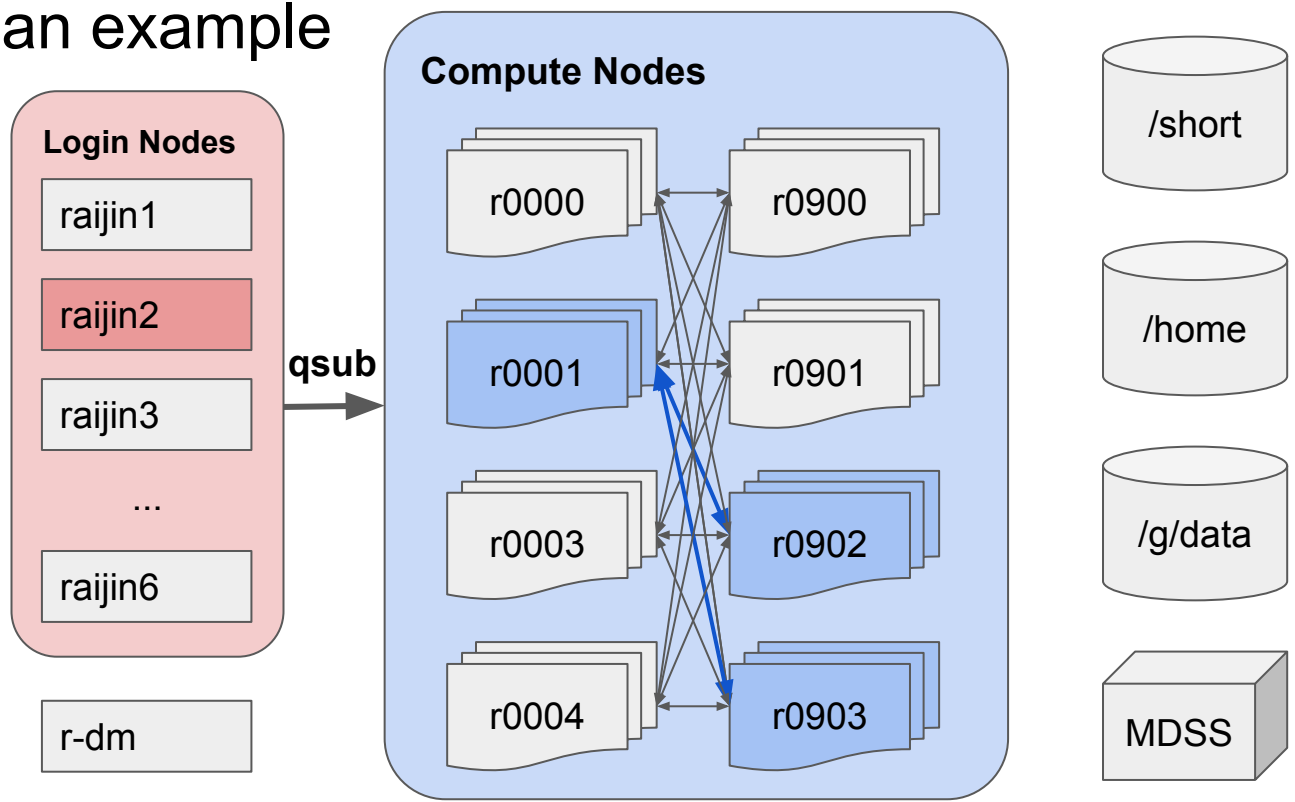
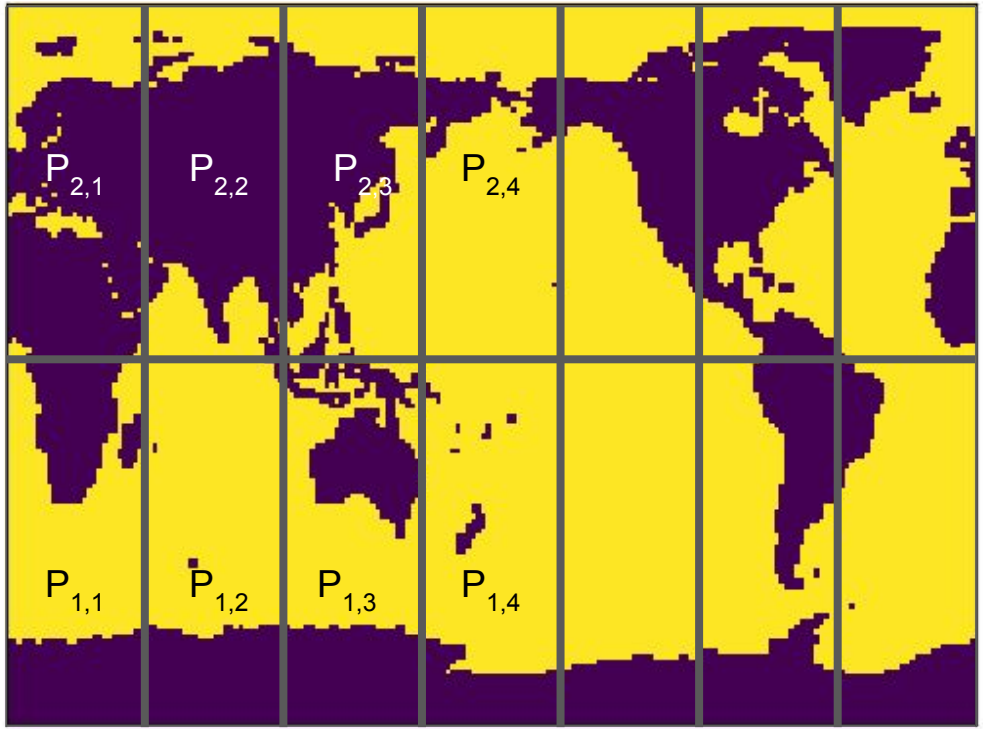
Supercomputers architecture:

Raijin as an example

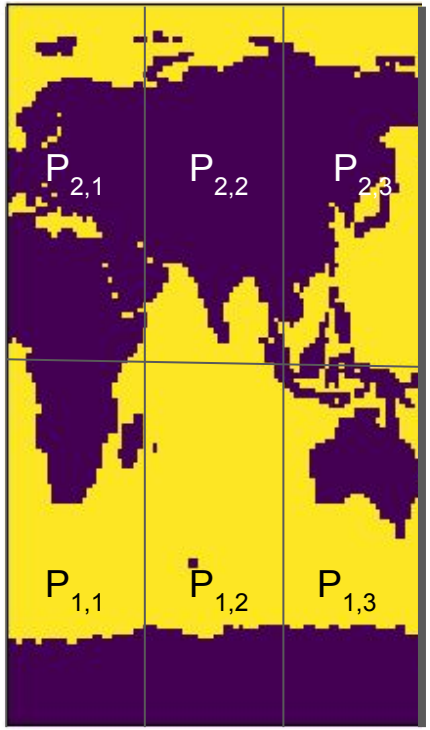


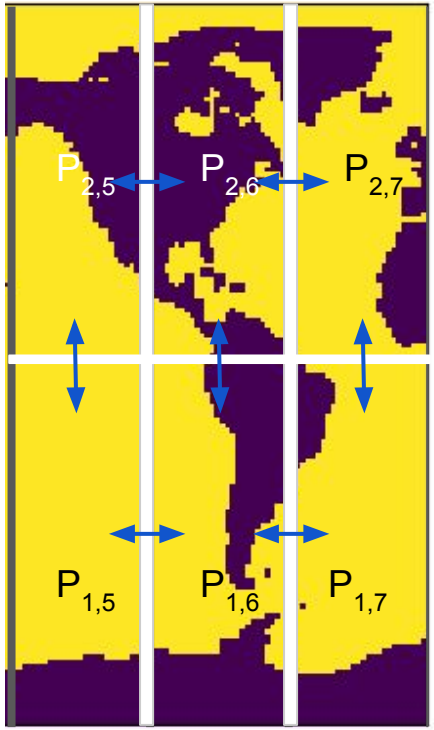
Decomposition



Parallelisation

Shared Memory





Distributed Memory

Shared Memory (OpenMP)

```
!$OMP PARALLEL DO SHARED(u, dudt)
do j=0, nj
  do i=0, ni
    du2dx2 = (u[i+1,j] - 2*u[i,j]
              + u[i-1,j])/deltax**s
    du2dy2 = (u[i,j+1] - 2*u[i,j]
              + u[i,j-1])/deltay**2

    dudt[i,j] = alpha*(du2dx2 +
                       du2dy2)
  end do
end do
!$OMP END PARALLEL DO
```

Each processor has access to the same memory

Specific sections are marked as parallel - e.g. loops

Variables can be either shared so all threads see the same data, or private so each thread has a different variable

Distributed Memory (MPI)

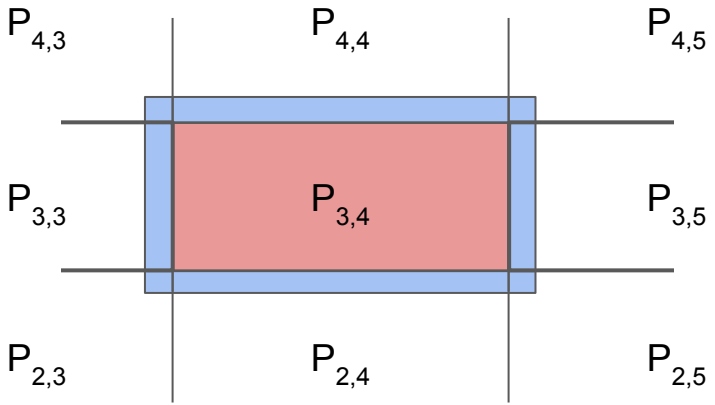
```
call halo_exchange(u, MPI_COMM_WORLD)

do j=local_j0, local_nj
  do i=local_i0, local_ni
    du2dx2[i,j] = (u[i+1,j] - 2*u[i,j]
                + u[i-1,j])/deltax**s
    du2dy2[i,j] = (u[i,j+1] - 2*u[i,j]
                + u[i,j-1])/deltay**2

    dudt[i,j] = alpha * (du2dx2[i,j]
                + du2dy2[i,j])
  end do
end do
```

Each processor's data is kept separate

Neighbouring data is kept as a "halo" around each field



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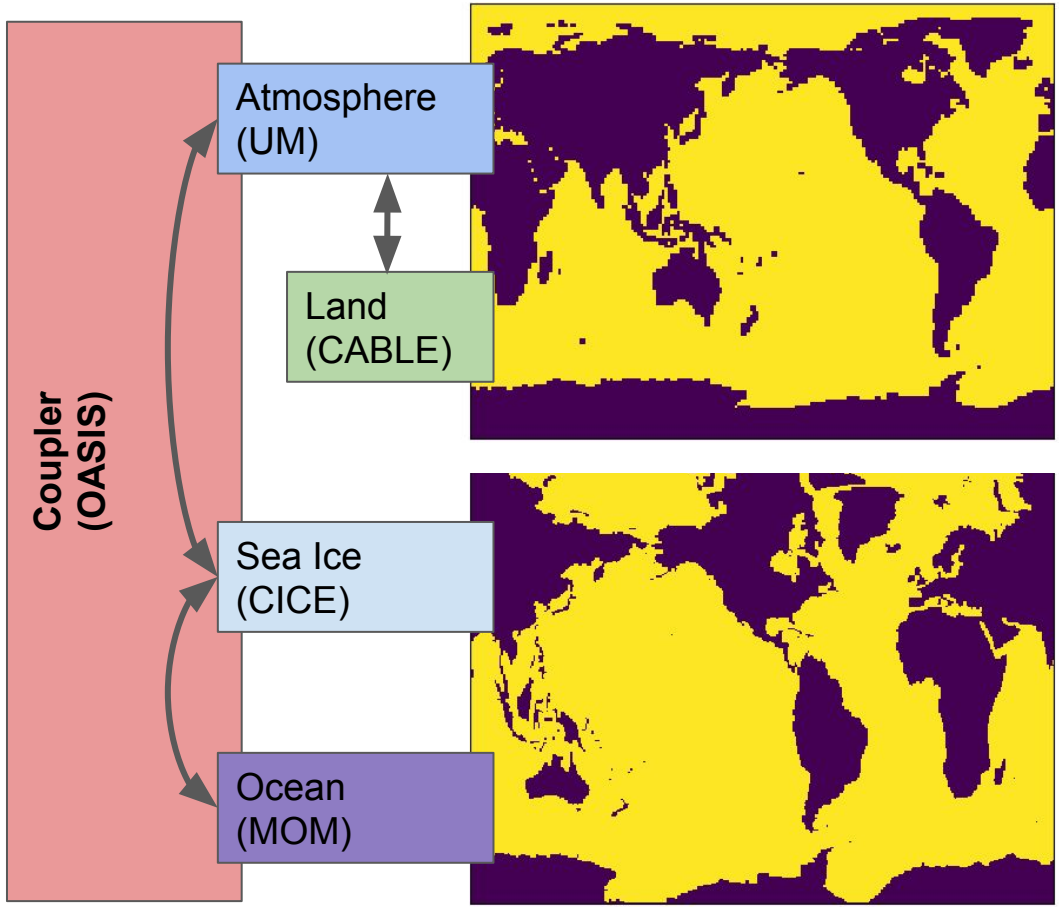
Coupling


Coupler
(OASIS)
Atmosphere
(UM)
Land
(CABLE)
Sea Ice
(CICE)
Ocean
(MOM)
Atmosphere
Grid
Ocean
Grid

Optimisation

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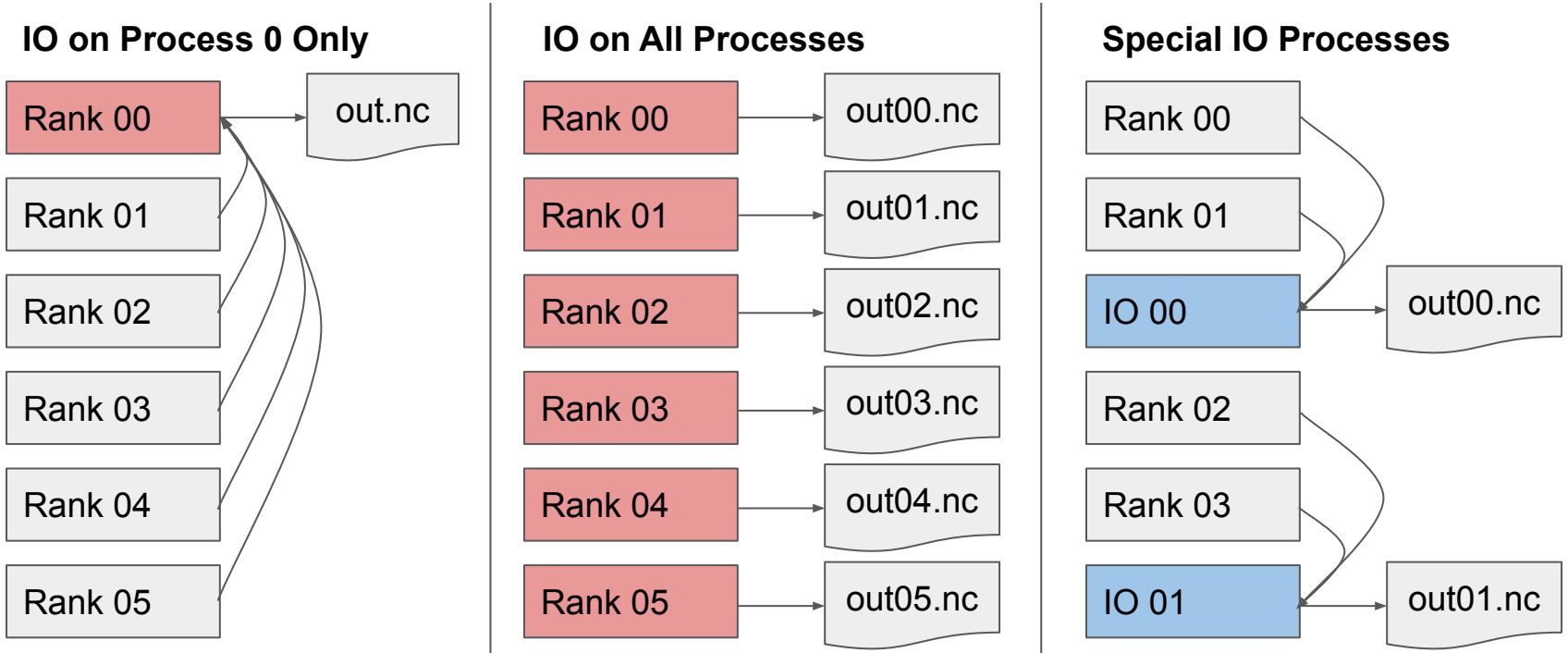
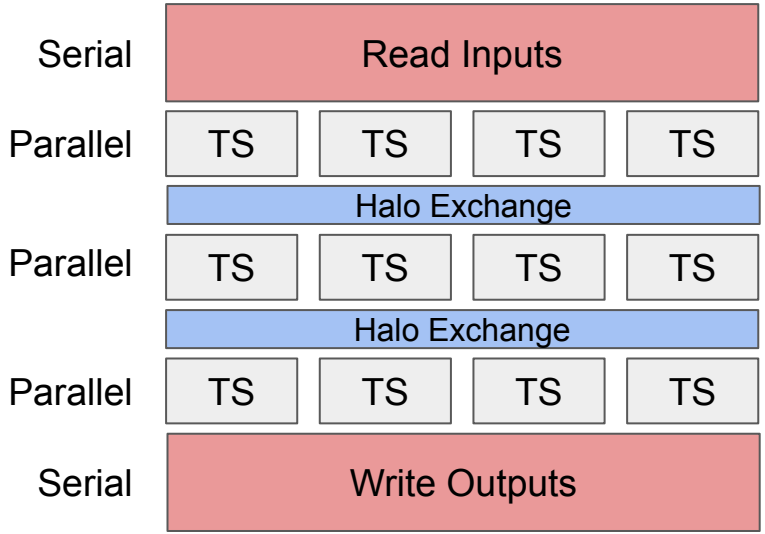
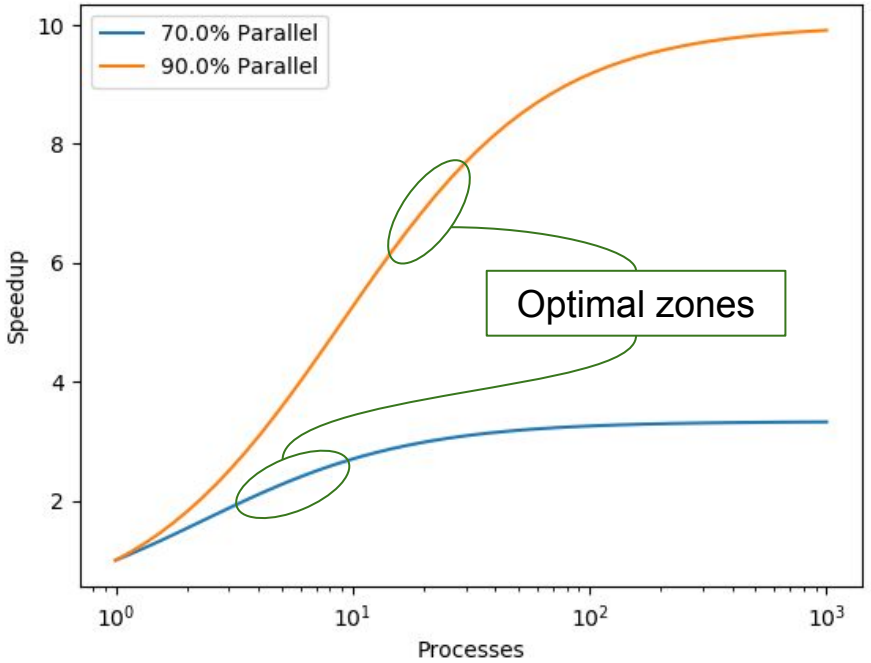
IO Strategies



Scaling

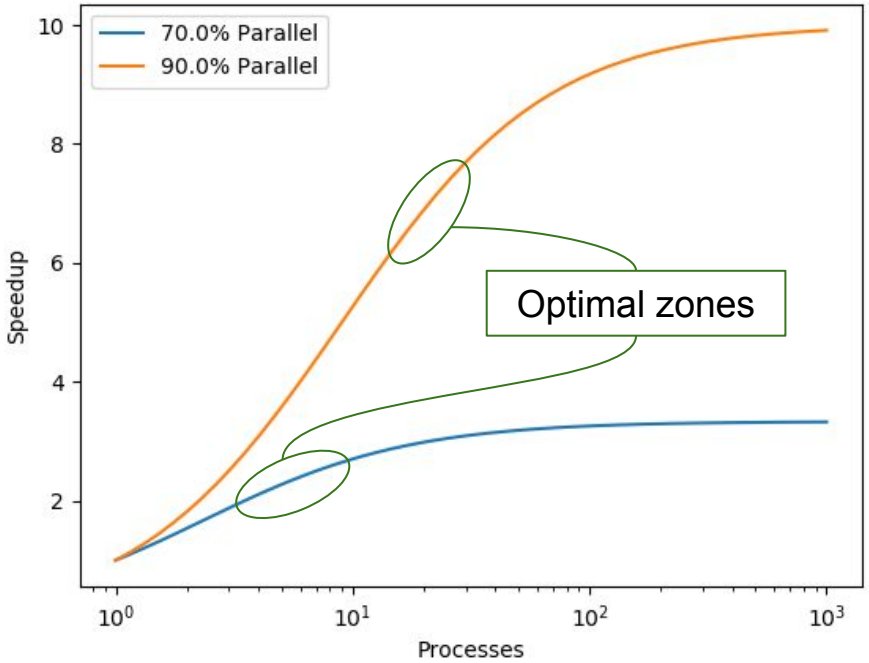




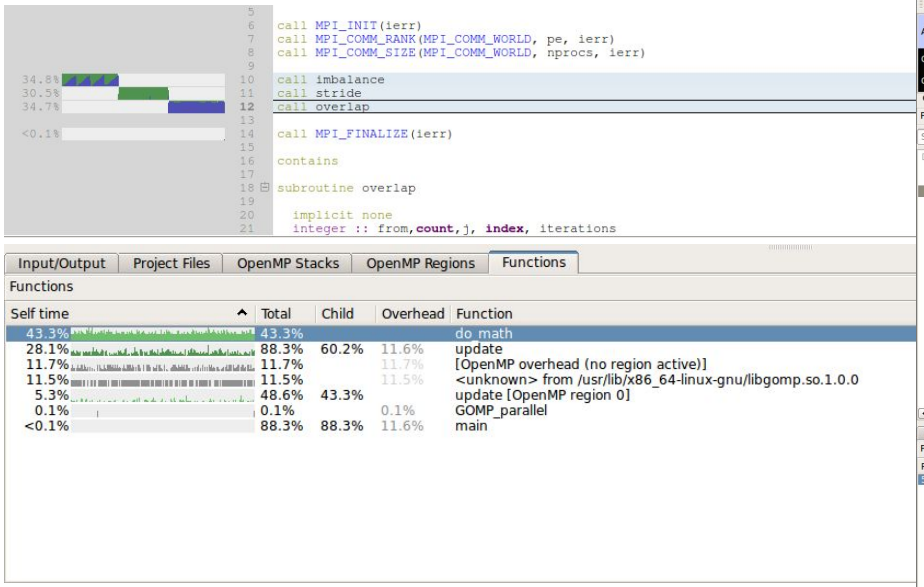
Optimising Efficiency

Experiment with short model runs

Optimise **(SU cost x walltime)** for different numbers of CPUs to find the best efficiency for your experiment

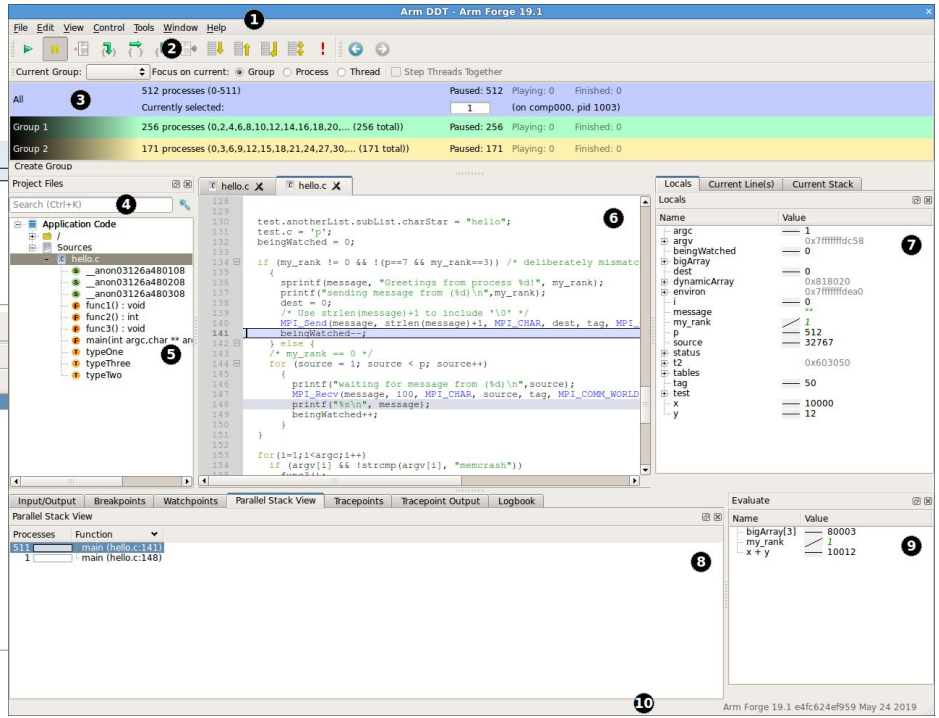


Profilers…



https://www.arm.com

and Debuggers



Model Output

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Data Publishing

FAIR Principles

Findable - DOI, metadata

Accessible - Standard formats

Interoperable - Common vocabularies

Reusable - Provenance, licence

NCI Data Catalogue

https://geonetwork.nci.org.au

Research Data Australia Catalogue

https://researchdata.ands.org.au/

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NetCDF

```
netcdf
tas_Amon_ACCESS1-0_historical_r1i1p1_185001-200512 {
 dimensions:
    time = UNLIMITED ; // (1872 currently)
    lat = 145 ;
    lon = 192 ;
variables:
   double time(time) ;
          time:units = "days since 0001-01-01" ;
          time:calendar = "proleptic_gregorian" ;
          time:standard_name = "time" ;
    float tas(time, lat, lon) ;
          tas:standard_name = "air_temperature" ;
          tas:long_name = "Near-Surface Air Temperature" ;
          tas:units = "K" ;
          tas:cell_methods = "time: mean" ;
          tas:cell_measures = "area: areacella" ;
// global attributes:
          :source = "ACCESS1-0 2011." ;
```

Climate and Forecasting Conventions
cfconventions.org

ncdump -h - Show metadata

cdo, nco - Stats, climate metrics, regridding

libnetcdf, libnetcdff - C and Fortran libraries

xarray, iris - metadata-aware Python libraries

Files can be read over the internet with THREDDS/OpenDAP

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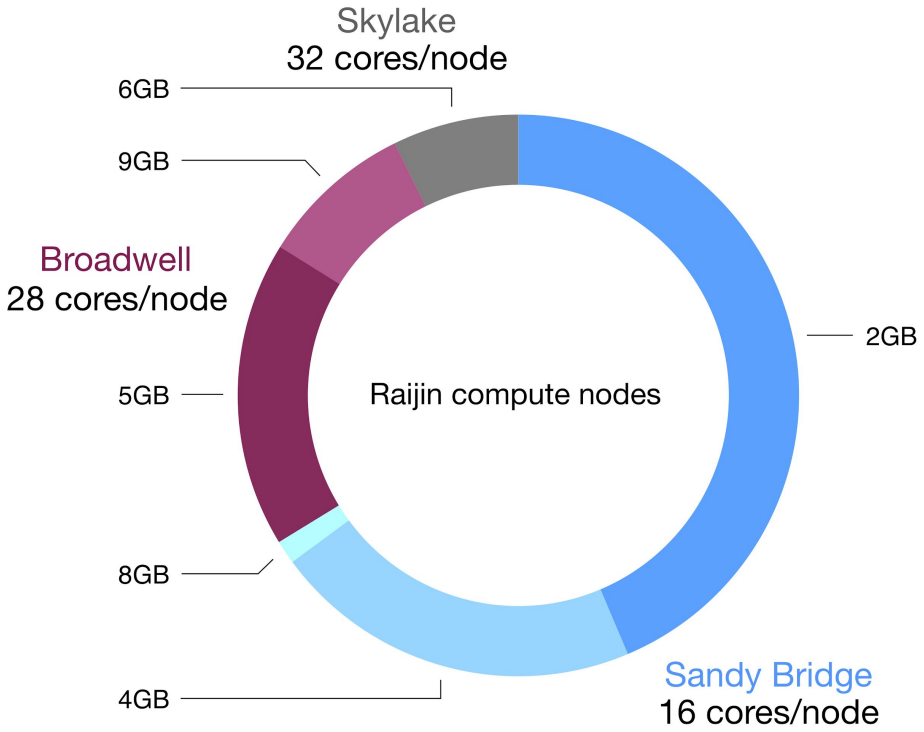
NCI Raijin

Raijin Nodes



Special Nodes:

- **gpu**: 32 nodes with GPUs
- **hugemem**: 10 nodes with 1TB memory
- **knl**: 32 nodes with Knights Landing CPUs

Tenjin (Openstack Cloud)

- 100 16-core nodes
- Access to /g/data filesystems

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Submitting jobs: PBSPro Scheduler

```
#!/bin/bash
#PBS -q normal
#PBS -l cpus=16
#PBS -l mem=32gb
#PBS -l walltime=01:00:00
#PBS -l wd

module load openmpi

mpirun ./wrf.exe
```

`qsub` - Submit a job

`qstat -U $USER` - See your jobs

`nqstat -P $PROJECT` - Project jobs

qdel $JOBID - Stop a job

qcat $JOBID - See job output

MPI programs get the number of processes from the queue system

Queues

normal - 1 SU / cpu / wall hour
normalbw - 1.25 SU / cpu / wall hour
normalsl - 1.5 SU / cpu / wall hour

express - 3 SU / cpu / wall hour
expressbw - 3.75 SU / cpu / wall hour

copyq - 1 SU / cpu / wall hour
Max of 1 cpu per job
Access to internet for file downloads/ uploads

hugemem - 1.25 SU / cpu / wall hour
gpu - 3 SU / cpu / wall hour
knl - 0.25 SU / cpu / wall hour

Storage

/home
- Backed up
- 2 GB / user

/short/$PROJECT
- Shared per-project quota
- Short-term storage
- /short/public for sharing files

/g/data/$PROJECT
- Shared per-project quota
- Medium-term storage
- Cloud access

MDSS (Tape storage)
- Shared per-project quota
- Slow access
- Long-term archival
- Redundant (2 sites)
- **mdss** command to access

$PBS_JOBFS (Node storage)
- Storage directly on the node
- Disappears after a job completes

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Central Dataset Storage

Reanalyses

- **ERA5, ERA-Interim**
- **JRA55**
- **OSTIA-SST**

Intercomparisons

- **CMIP5**
- **CMIP6**

Rainfall

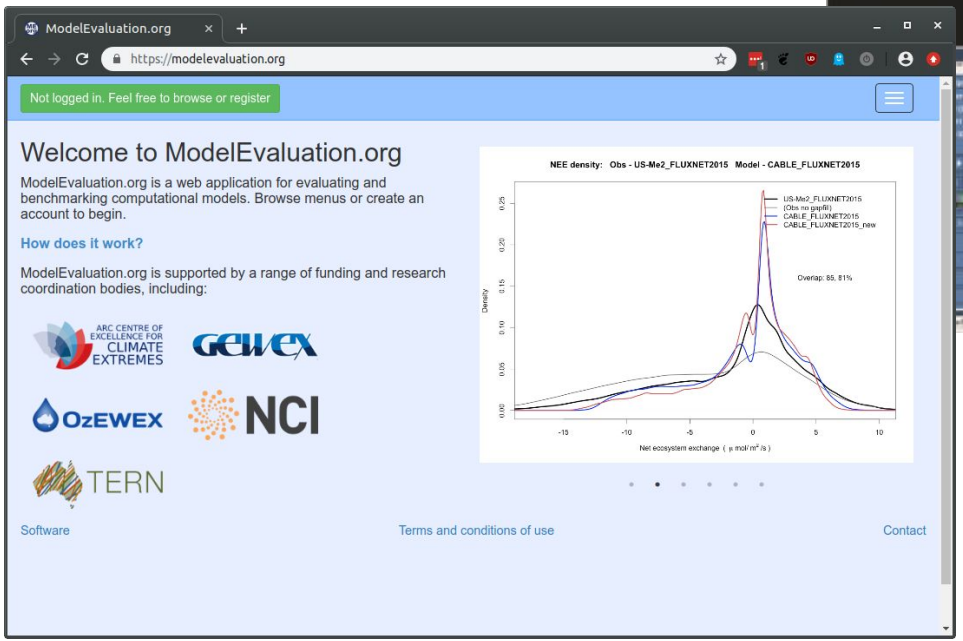
- **TRMM**
- **AWAP/AGCD**
- **Open Radar**

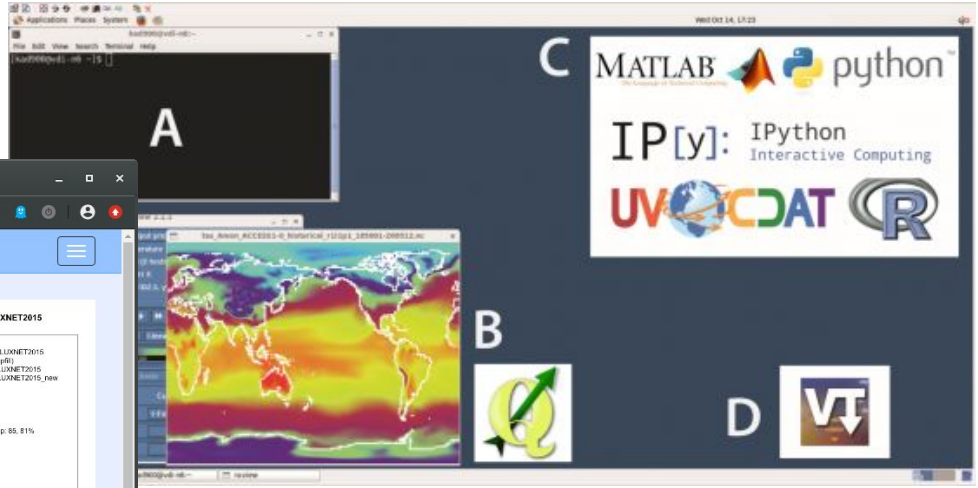
Centrally downloaded / published datasets are outside of the CLEX storage quota

You can request useful datasets by emailing us at **cws_help@nci.org.au**

http://climate-cms.wikis.unsw.edu.au/Category:Dataset

Cloud Computing





CLEX Resources at NCI

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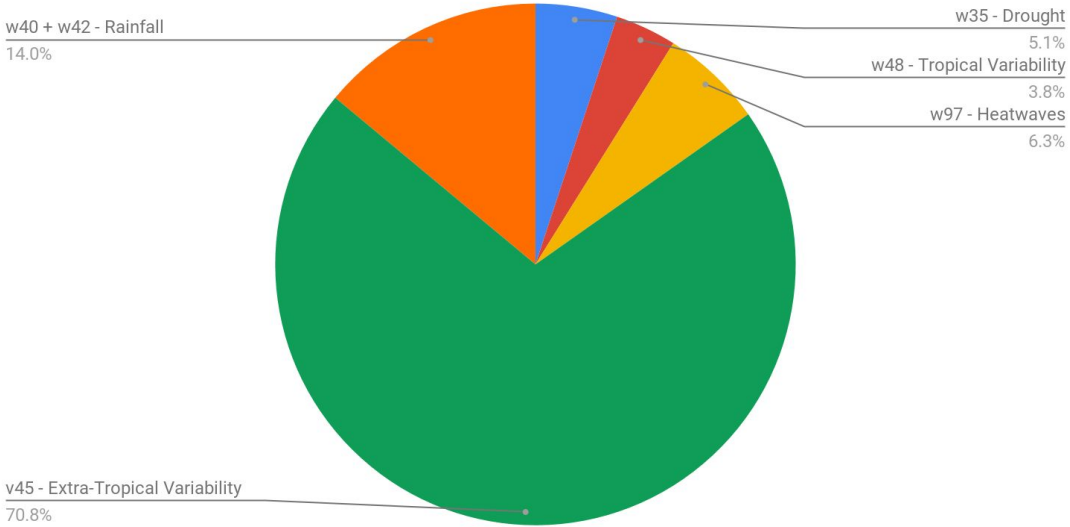
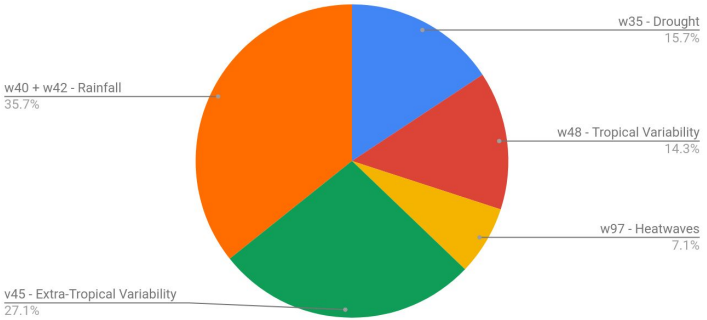
CLEX Resources

Shared between projects: v45, w35, w40, w42, w48, w97

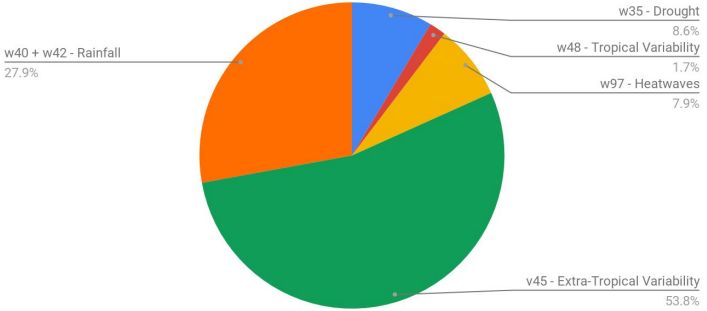
SU - Approx 3.1 MSU / quarter



/g/data Disk - 0.42 PB



MDSS Tape - 0.75 PB



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NCI Projects

w35 - Drought

w40 - Rainfall (Lane)

w42 - Rainfall (Sherwood)

v45 - Extra-Tropical Variability

w48 - Tropical Variability

w97 - Heatwaves

Join projects at

https://my.nci.org.au

ua8 - Publication Storage
hh5 - LIEF Storage
access - ACCESS model input data

+ projects for specific datasets

http://climate-cms.wikis.unsw.edu.au/Category:Dataset

Managing Allocations

nci_account - Current allocation and usage

short_files_report - Project disk usage by user
gdata1_files_report, …

lquota - Storage limits

nf_limits - Maximum queue resources

CMS Conda environment tools

```
module use /g/data3/hh5/public/modules
module load conda/analysis3
```

ncimonitor - Graphs of per-project compute and data usage

nccompress - Compress NetCDF files under a directory

More Info

CLEX CMS

wiki	- climate-cms.wikis.unsw.edu.au
training	- weekly over VC
email	- cws_help@nci.org.au
chat	- arccss.slack.com

NCI

web	- nci.org.au
docs	- opus.nci.org.au
email	- help@nci.org.au






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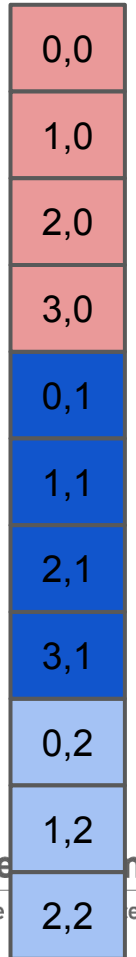
Memory Layout

Model Field

0,0	0,1	0,2	0,3
1,0	1,1	1,2	1,3
2,0	2,1	2,2	2,3
3,0	3,1	3,2	3,3

Computer Memory



Raijin Nodes

Sandy Bridge (**normal**/**express**):
- 3503 nodes
- 16 cpus/node
- 32, 64, 128 GB memory/node (16:8:1)

Broadwell (**normalbw**/**expressbw**):
- 814 nodes
- 28 cpus/node
- 128, 256 GB memory/node (2:1)

Skylake (**normalsl**):
- 192 nodes
- 32 cpus/node
- 192 GB memory/node

Special Nodes:
- **gpu**: 32 nodes with GPUs
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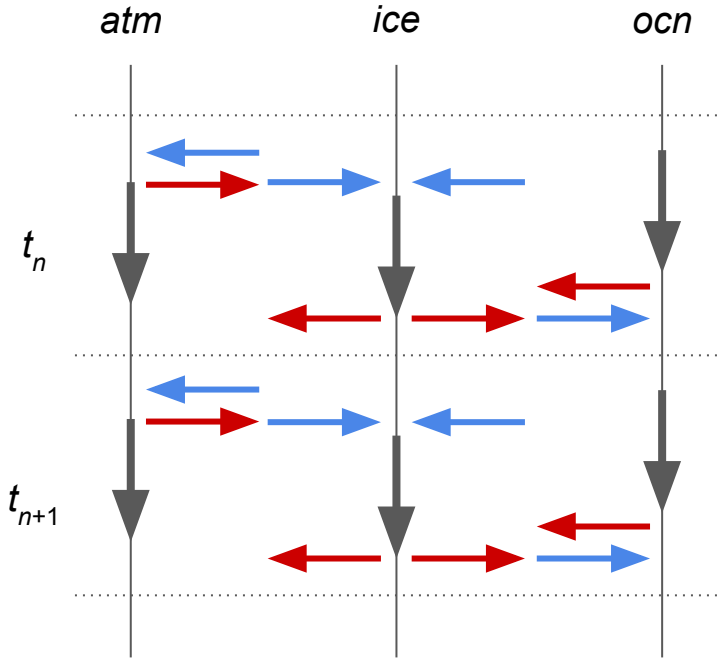
Coupling



Coupling (test other slide format)