Multi-scale CAFE framework for simulating fracture in heterogeneous materials implemented in Fortran coarrays and MPI

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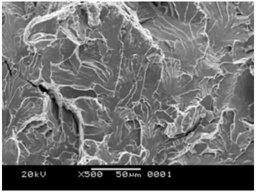
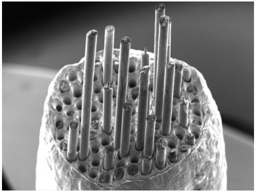
Fracture in heterogeneous materials



polycrystal cleavage

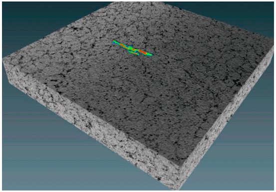
reinforced concrete

CFRP



metal matrix

bone

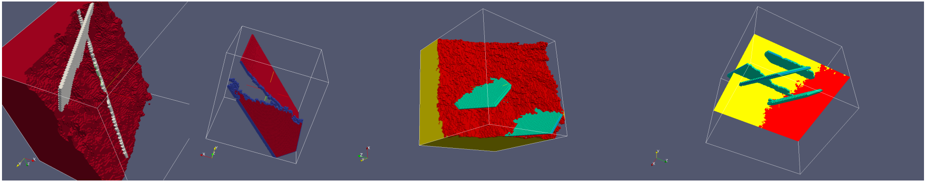


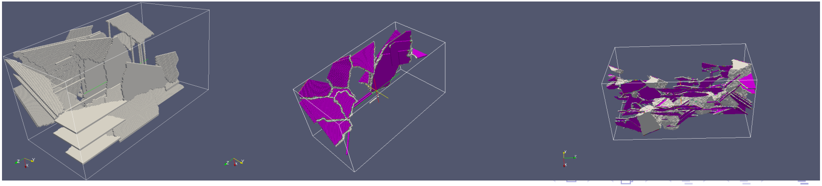
graphite

- All real materials are heterogeneous
- Multiple fracture and damage processes happen at different time and length scales → need multi-scale framework

Fracture: CA + FE = CAFE multi-scale model ▸ CGPACK

- Structured grids - cellular automata (CA), unstructured grids - finite elements (FE)
- CA (microstructure) + FE (continuum mechanics) = CAFE
- Transgranular cleavage - fracture stress or strain criteria
- FE → CA (localisation) - stress, strain fields
- CA → FE (homogenisation) - damage variables



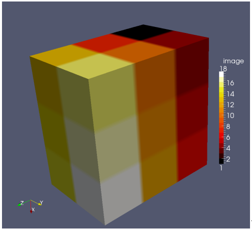


Fortran coarrays for CA

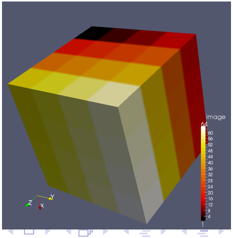
- Fortran native SPMD parallel programming feature
- Fortran standard since 2008. More features in 2015.
- Cray, Intel, OpenCoarrays/GCC support
- CGPACK - cellular automata microstructure simulation library: cgpack.sf.net. See also [1, 2, 3].
- Easy halo exchange
- CA space coarray - 4D array, 3 codimensions:

```
integer, allocatable :: space(:,:,:,:)[:,:,:]
```

- Ideal for structured grids:

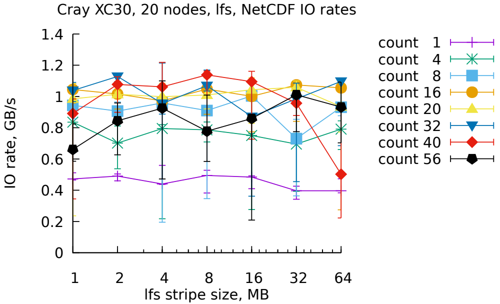


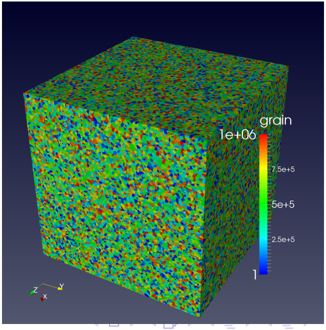
← 18 imgs; 64 imgs →



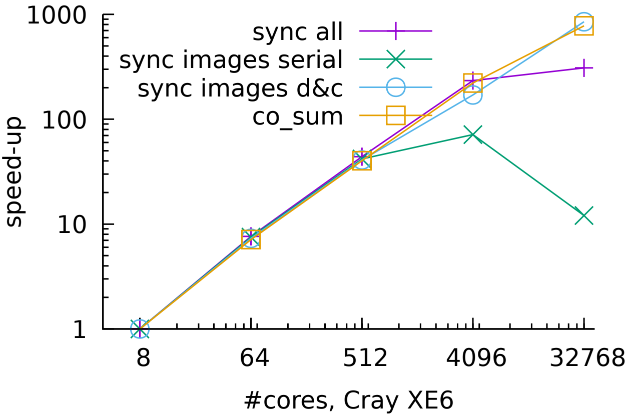
Coarray IO - no native Fortran parallel IO

- MPI/IO up to 2.3GB/s on Cray XE6 ▸ BCS talk
- MPI/IO up to 8GB/s on Cray XC30 (can reach 14GB/s [4])
- NetCDF 4.3, HDF5 1.8.14 - only up to 1.2GB/s on Cray XC30.
- lfs stripe count, size, number of images, file size, Cray hugepages...
- 0.5 - 1TB datasets





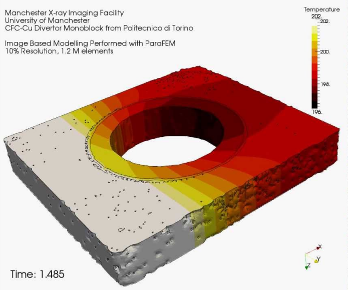
CGPACK solidification scaling

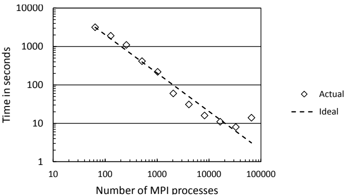


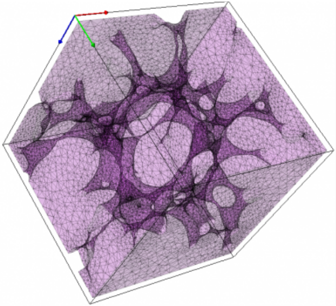
Scaling varies for different programs built with CGPACK, depending on which routines are called, in what order and requirements for synchronisation.

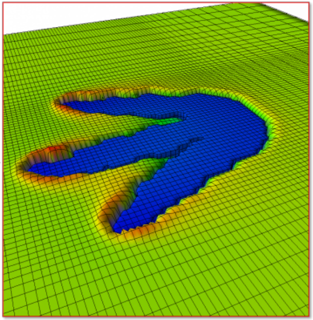
ParaFEM - scalable general purpose finite element library

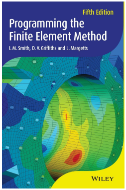
- `http://parafem.org.uk`
- Fortran 90 MPI
- Highly portable, many users [5]
- Excellent scaling
- BSD license



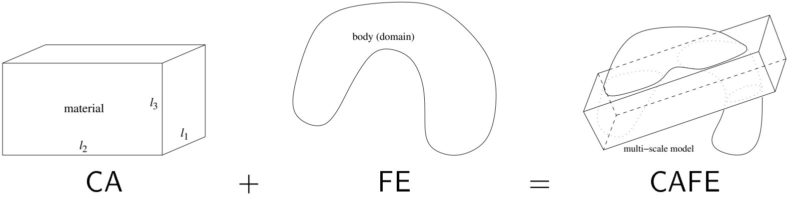


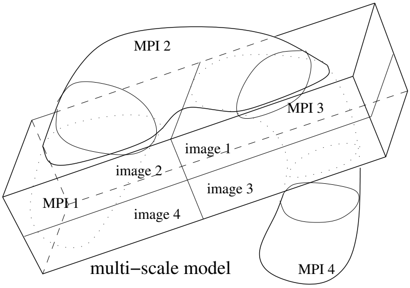


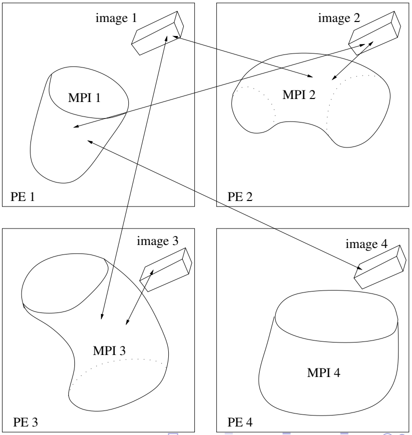




CAFE design: structured CA grid + unstructured FE grid







Example with 4 PE (4 MPI processes, 4 coarray images). Arrows are FE $\leftrightarrow$ CA comms.

FE → CA mapping via a private allocatable array of derived type:

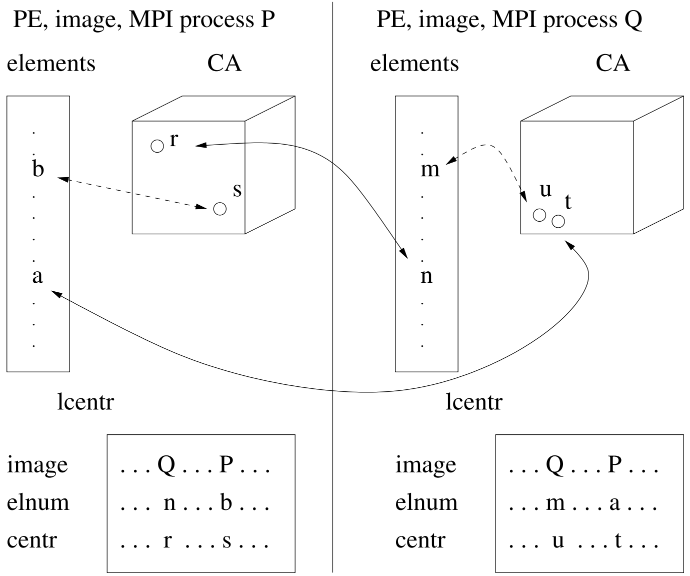
```
type mcen
  integer :: image, elnum
  real :: centr(3)
end type mcen
type( mcen ), allocatable :: lcentr(:)
```

based on coordinates of FE centroids calculated by each MPI process and stored in centroid_tmp coarray:

```
type rca
  real, allocatable :: r(:,:)
end type rca
type( rca ) :: centroid_tmp[*]
 :
allocate( centroid_tmp%r(3, nels_pp) )
```

where nels_pp is the number of FE stored on this PE.

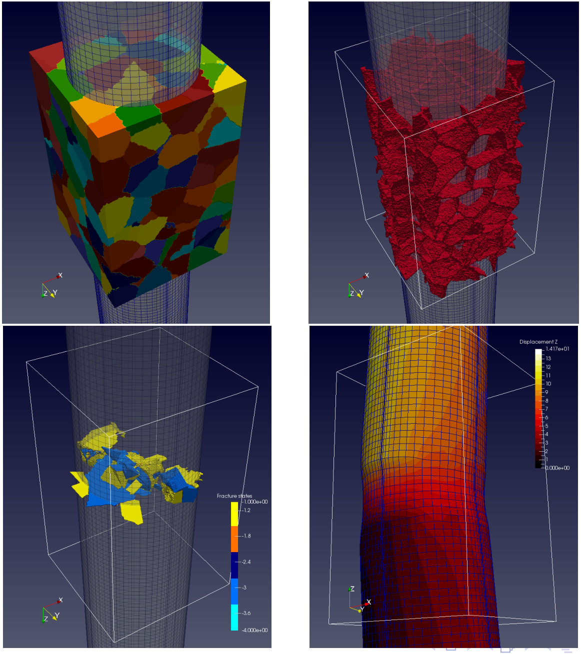
lcentr arrays on images P and Q



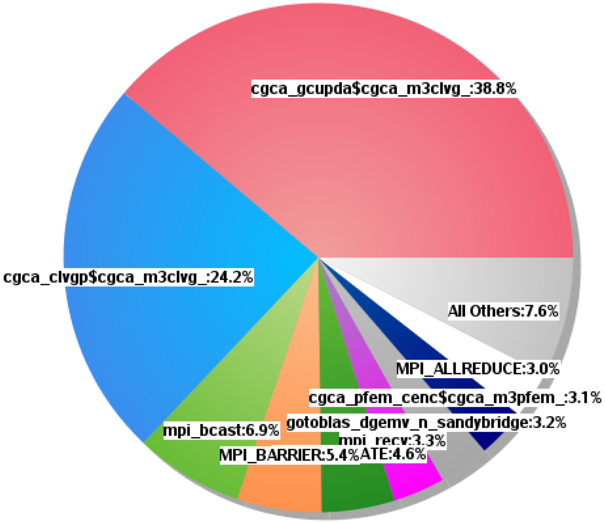
Fracture modelling

- Diverse CAFE fracture models can be constructed from CGPACK + ParaFEM libraries.
- Simple case: isotropic linear elastic FE (E, ν) + cleavage (fully brittle transgranular fracture mode) CA.
- FE stress tensor $\mathbf{t}$ passed to CA, resolved on normal stresses on $\{100\}$ and $\{110\}$ crystal planes - t_{100}, t_{110} [1, 6].
- 2 parameters - fracture stress, σ_F, linked to the free surface energy, γ, and a characteristic length, L.
- If $t_{100} \geq \sigma_F$ or $t_{110} \geq \sigma_F$ then a CA crack extends by L per unit of time.
- Crack morphology is reduced to a single damage variable, d. $d = 1$ initially (no damage). $d = 0$ - integration point has failed, no load bearing capacity.

Cleavage in a steel cylinder under tension



CrayPAT profiling 1



Profiling function distribution for ParaFEM/CGPACK MPI/coarray miniapp with all-to-all routine cgca_gcupda at 7200 cores.

CrayPAT profiling 2

```
100.0% | 20,520.4 |    -- |     -- |Total
|-------------------------------------------------------------
|  71.4% | 14,649.9 |    -- |     -- |USER
||------------------------------------------------------------
||  38.7% |  7,950.6 | 913.4 | 10.3% |cgca_gcupda$cgca_m3clvg_
||  24.1% |  4,951.2 | 940.8 | 16.0% |cgca_clvgp$cgca_m3clvg_
||   3.1% |    638.0 |  70.0 |  9.9% |cgca_pfem_cenc$cgca_m3pfem_
||   1.8% |    367.5 | 578.5 | 61.2% |cgca_hxi$cgca_m2hx_
||   1.7% |    346.0 | 196.0 | 36.2% |cgca_clvgn$cgca_m3clvg_
||============================================================
|  19.8% |  4,061.4 |    -- |     -- |MPI
||------------------------------------------------------------
||   6.9% |  1,413.5 | 356.5 | 20.1% |mpi_bcast
||   5.4% |  1,098.3 | 419.7 | 27.7% |MPI_BARRIER
||   3.3% |    670.0 | 322.0 | 32.5% |mpi_recv
||   3.0% |    615.3 |  61.7 |  9.1% |MPI_ALLREDUCE
||============================================================
|   8.8% |  1,797.2 |    -- |     -- |ETC
||------------------------------------------------------------
||   4.6% |    950.5 |   5.5 |  0.6% |__DEALLOCATE
||   3.2% |    654.2 | 110.8 | 14.5% |gotoblas_dgemv_n_sandybridge
|=============================================================
```

Raw profiling data for ParaFEM/CGPACK MPI/coarray miniapp with all-to-all routine cgca_gcupda at 7200 cores.

cgca_gcupda - all-to-all

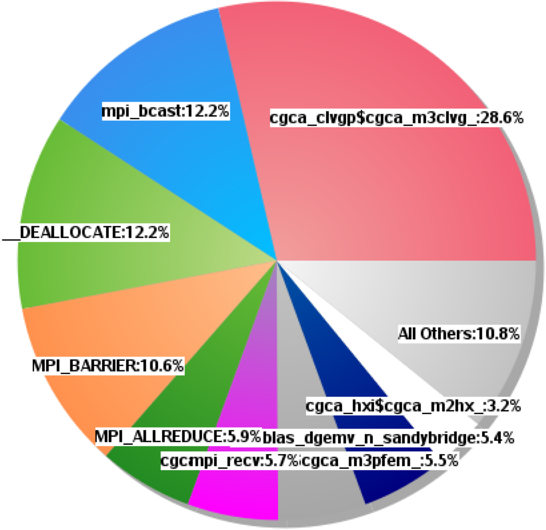
```
integer :: gcupd(100,3)[*], rndint, j, &
           img, gcupd_local(100,3)
real :: rnd
:
call random_number( rnd )
rndint = int( rnd*num_images() ) + 1
do j = rndint, rndint + num_images() - 1
 img = j
 if (img .gt. num_images()) &
      img = img - num_images()
  if (img .eq. this_image()) cycle
  :
  gcupd_local(:,:) = gcupd(:,:)[img]
  :
end do
```

cgca_gcupdn - nearest neighbour

```
do i = -1 , 1
do j = -1 , 1
do k = -1 , 1
 ! Get the coindex set of the neighbour
 ncod = mycod + (/ i, j, k /)
 :
 gcupd_local(:,:) = &
     gcupd(:,:)[ncod(1),ncod(2),ncod(3)]
 :
end do
end do
end do
```

Note: the nearest neighbour must be called *multiple times* to propagate changes from every image to all other images.

CrayPAT profiling cgca_gcupdn



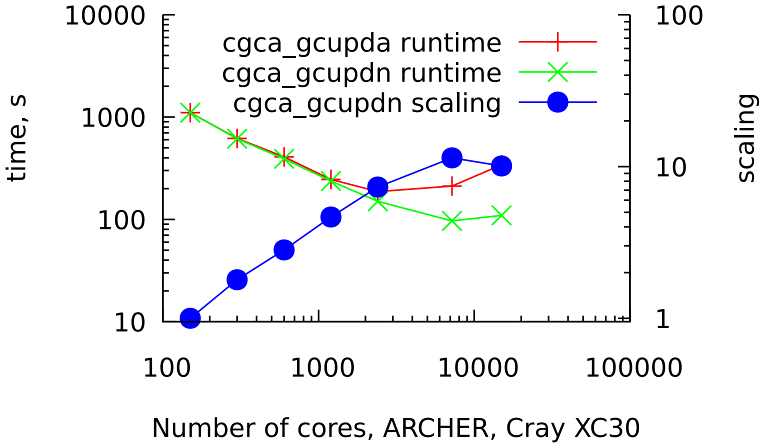
Profiling function distribution for ParaFEM/CGPACK MPI/coarray miniapp with the nearest neighbour routine cgca_gcupdn at 7200 cores.

CrayPAT profiling cgca_gcupdn

```
100.0% | 12,199.5 |     -- |     -- |Total
|-----------------------------------------------------------------
|  44.8% |  5,459.7 |     -- |     -- |USER
||----------------------------------------------------------------
||  28.6% |  3,484.0 | 582.0 | 14.3% |cgca_clvgp$cgca_m3clvg_
||   5.5% |    666.1 |  93.9 | 12.4% |cgca_pfem_cenc$cgca_m3pfem_
||   3.2% |    393.1 | 752.9 | 65.7% |cgca_hxi$cgca_m2hx_
||   2.8% |    346.0 | 176.0 | 33.7% |cgca_clvgn$cgca_m3clvg_
||   1.4% |    165.2 |  37.8 | 18.6% |cgca_sld$cgca_m3sld_
||   1.0% |    126.0 |  82.0 | 39.4% |xx14_
||================================================================
|  36.7% |  4,472.1 |     -- |     -- |MPI
||----------------------------------------------------------------
||  12.2% |  1,484.4 | 380.6 | 20.4% |mpi_bcast
||  10.6% |  1,287.9 | 389.1 | 23.2% |MPI_BARRIER
||   5.9% |    714.9 |  90.1 | 11.2% |MPI_ALLREDUCE
||   5.7% |    689.4 | 338.6 | 32.9% |mpi_recv
||   1.5% |    179.1 | 417.9 | 70.0% |MPI_REDUCE
||================================================================
|  18.5% |  2,256.1 |     -- |     -- |ETC
||----------------------------------------------------------------
||  12.1% |  1,480.9 |   4.1 |  0.3% |__DEALLOCATE
||   5.4% |    653.8 |  95.2 | 12.7% |gotoblas_dgemv_n_sandybridge
|=================================================================
```

Raw profiling data for ParaFEM/CGPACK MPI/coarray miniapp with the nearest neighbour routine cgca_gcupdn at 7200 cores.

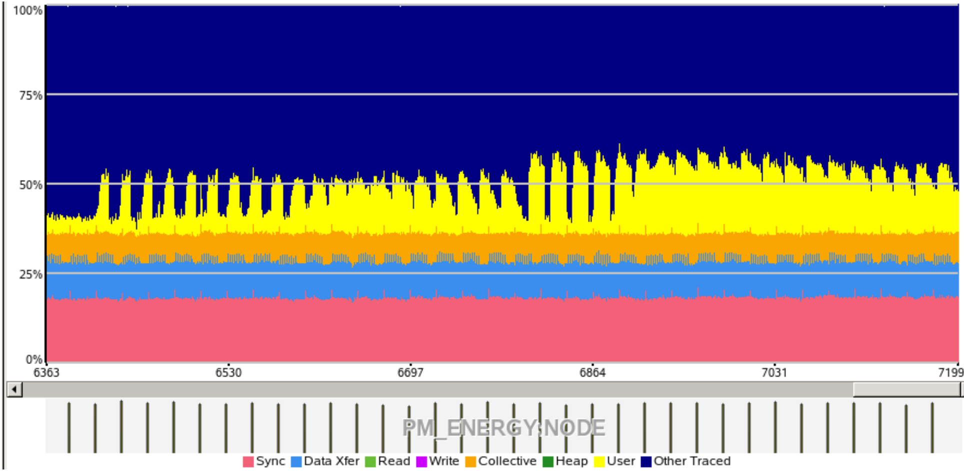
Scaling improvement with cgca_gcupdn over cgca_gcupda



Runtimes and scaling for ParaFEM/CGPACK MPI/coarray miniapp with the nearest neighbour, cgca_gcupdn, and all-to-all, cgca_gcupda, algorithms.

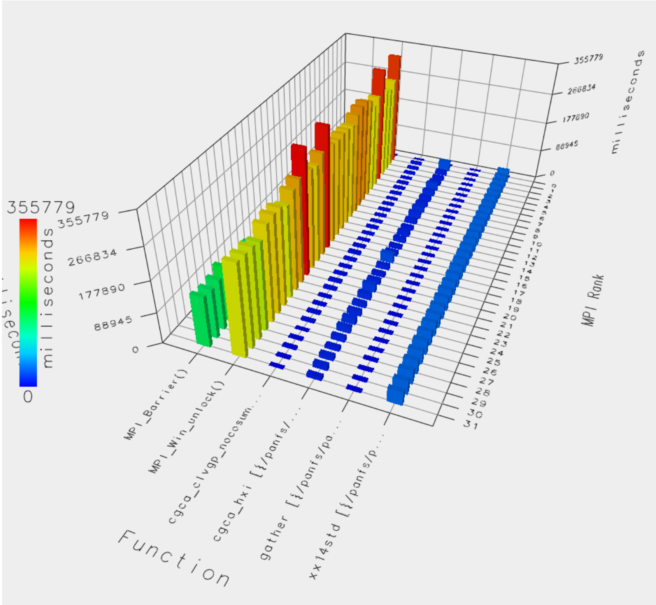
Scaling limit increased from 2k to 7k cores.

CrayPAT - load imbalance on 7k cores on Cray XC30



Whole program activity, shown in % total time per process.
Processes 6363 to 7199 are shown.

TAU profiling: Intel 16 coarray implementation - MPI RMA



2x 16-core nodes, 32 images. Poor optimisation? ▸ TAU

CA - coarray (over)synchronisation?

```
call cgca_nr( space )  ! sync all inside
call cgca_rt( grt )    ! sync all inside
call cgca_sld( space ) ! sync all inside
call cgca_igb( space )
sync all
call cgca_hxi( space )
sync all
call cgca_gbs( space )
sync all
call cgca_hxi( space )
sync all
call cgca_gcu( space ) ! local routine no sync
```

- All images sync with their 26 neighbours.
- Some routines have sync inside.
- Other sync responsibility is left to end user.

Fortran 2015 events: more flexible than SYNC IMAGES [7]

```
use, intrinsic iso_fortran_env, only:event_type
type(event_type) :: var[:,:,:]
integer, allocatable :: space(:,:,:,:)[:,:,:]
integer :: errstat, myrank(3)
! allocate var, space
myrank = this_image( space )
! do some work, then notify neighbours
event post(var[myrank(1)-1,myrank(2),myrank(3)], &
   stat=errstat)
! 25 more posts
:
event wait(var, until_count=26, stat=errstat)
! when all 26 neighbours posted, continue work
:
```

Future: thread level parallelism: OpenMP, DO CONCURRENT

```
main: do iter = 1,N
 do x3 = lbr(3), ubr(3)
 do x2 = lbr(2), ubr(2)
 do x1 = lbr(1), ubr(1)
  live: if ...
   call cgca_clvgn( clvgflag )
   if ( clvgflag ) call sub( space )
  end if live
 end do
 end do
 end do
 call co_sum( clvgglob )
 sync all
 call cgca_hxi( space )
 sync all
 call cgca_dacf( space )
```

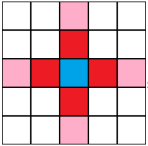
Conclusions

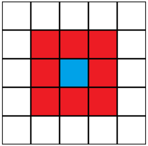
- Fortran coarrays are an ideal match for cellular automata
- Hybrid coarray+MPI multi-scale fracture framework is feasible
- Scaling up to 7k cores currently, work ongoing
- Profiling/tracing tools: CrayPAT, TAU, Score-P, Scalasca - coarray support is improving
- Coarray synchronisation - major issue: data integrity & performance

Acknowledgements

- This work was funded under the embedded CSE programme of the ARCHER UK National Supercomputing Service (http://www.archer.ac.uk), archer.ac.uk
- This work was carried out using the computational facilities of the Advanced Computing Research Centre, University of Bristol - https://www.acrc.bris.ac.uk, www.acrc.bris.ac.uk

Cellular automata (CA) basics

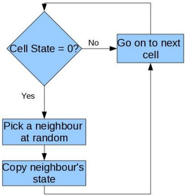
- discrete space, discrete time, discrete states - fully digital framework, structured grids
- finite or infinite space
- finite space: fixed or self-similar boundaries
- cell neighbourhood, e.g. von Neumann's: ,

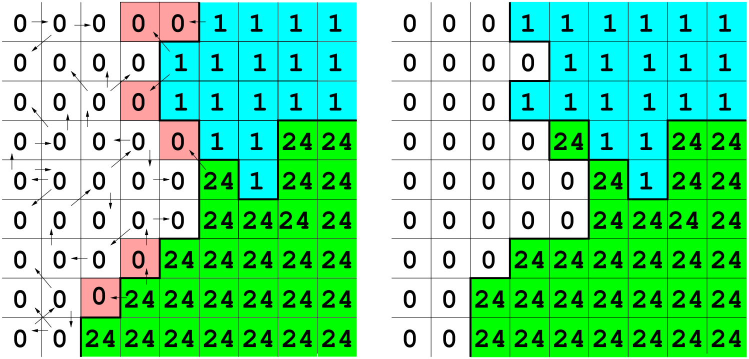
  or Moore's: 
- iterative process
- state of a cells at next iteration is a function of the state of this cells and of the states of its neighbourhood cells at the current iteration

▸ Wikipedia

Primitive 3D solidification - probabilistic CA

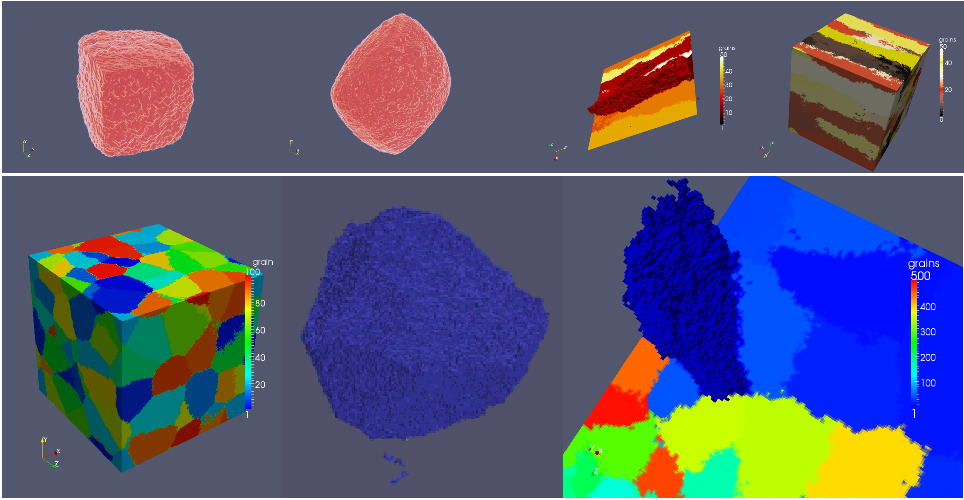
- States: liquid $= 0$, crystals > 0.
- Cell state uniquely encodes crystal orientation tensor, i.e. a look-up table.
- Each iteration a liquid cell acquires a state of a randomly chosen neighbour (3D Moore's neighbourhood - 26 cells).





i $\qquad\qquad$ $i + 1$

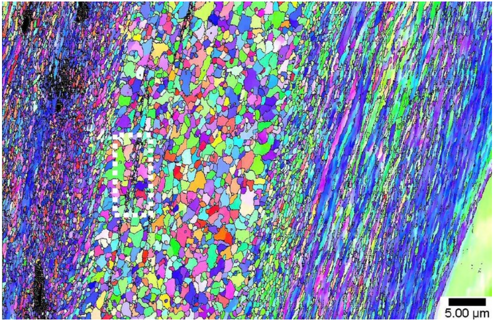
Primitive probabilistic 3D solidification - results

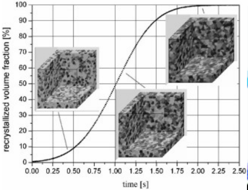


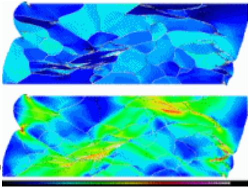
For more results ▸ CGPACK

Recrystallisation

- The grain boundary velocity $\dot{\mathbf{x}} = \mathbf{n}mp$, $\mathbf{n}$ - the normal to the grain boundary segment, m - mobility, p - the driving force.
- If $\dot{\mathbf{x}}\Delta t \geq c$, where Δt - time increment, c - cell size, then a cell joins the growing grain.
- Mobility strongly depends on temperature: $m \approx \alpha \exp\left(-\beta/T\right)$, α, β - some parameters, T - temperature.

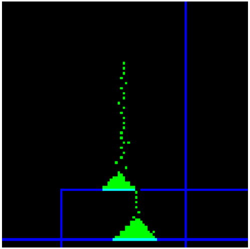




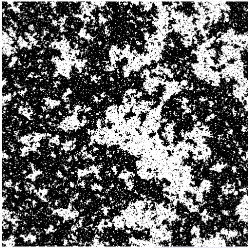


▸ Dierk Raabe site

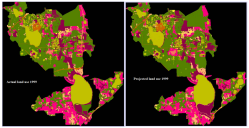
Other CA examples



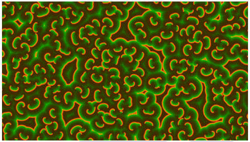
Sand pile formation



Ising magnetisation ▸ more info

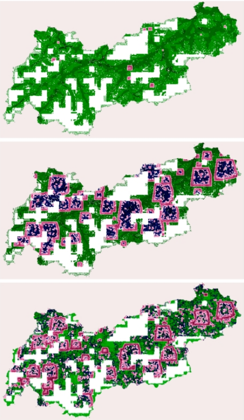


Land use ▸ more info



Diffusion ▸ animation ▸ info

Fire ▸ more info

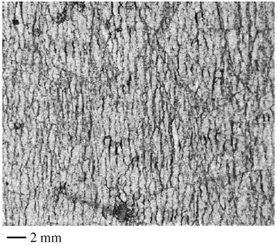


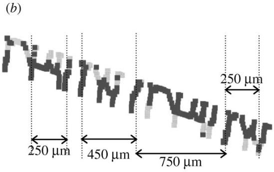
Epidemics, from The Open Med. Inform. J. 2(1):70-81, 2008.

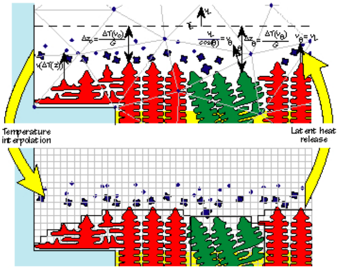
▸ PDF

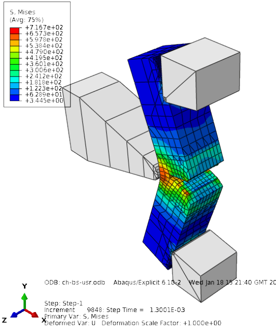
More CAFE examples

- Used for solidification [8], recrystallisation [9] and fracture [10, 11].
- FE - continuum mechanics - stress, strain, etc.
- CA - crystals, crystal boundaries, cleavage, grain boundary fracture
- FE → CA - stress, strain
- CA → FE - damage variables









Issues with CrayPAT

```
|  71.4% | 14,649.9 |     -- |     -- |USER
||-------------------------------------------------------------
||  38.7% |  7,950.6 | 913.4 | 10.3% |cgca_gcupda$cgca_m3clvg_
||  24.1% |  4,951.2 | 940.8 | 16.0% |cgca_clvgp$cgca_m3clvg_
||   3.1% |    638.0 |  70.0 |  9.9% |cgca_pfem_cenc$cgca_m3pfem_
||   1.8% |    367.5 | 578.5 | 61.2% |cgca_hxi$cgca_m2hx_
||   1.7% |    346.0 | 196.0 | 36.2% |cgca_clvgn$cgca_m3clvg_
||=============================================================
```

cgca_gcupda is top in sampling results, but is absent from tracing. It is called the same number of times as cgca_hxi.

```
|  29.7% |  99.743118 |         -- |    -- |  5,226,813.1 |USER
||-------------------------------------------------------------------------
||  17.4% |  58.326659 | 36.082315 | 38.2% |          5.0 |cgca_clvgp$cgca_m3clvg_
||   5.6% |  18.876152 |  5.062089 | 21.1% |          1.0 |cgca_pfem_cenc$cgca_m3pfem_
||   3.3% |  11.145318 | 15.328335 | 57.9% |          1.0 |xx14_
||   1.7% |   5.705317 |  8.788733 | 60.6% |  5,224,771.1 |cgca_clvgn$cgca_m3clvg_
||   1.7% |   5.689672 |  1.910819 | 25.1% |      2,035.0 |cgca_hxi$cgca_m2hx_
||=========================================================================
```

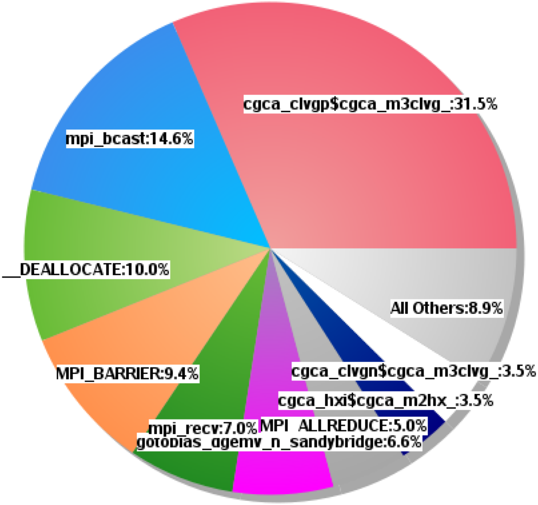
Issues with CrayPAT

All profiling was done with single thread.

```
CrayPat/X:  Version 6.2.2 Revision 13378 (xf 13240)  11/20/14 14:32:58
Number of PEs (MPI ranks):   480

Numbers of PEs per Node:      24  PEs on each of  20  Nodes

Numbers of Threads per PE:     3

Number of Cores per Socket:   12
Execution start time:  Thu Mar  3 13:40:17 2016
System name and speed:  tdsmom 2701 MHz
```

Incorrect number of threads identified by CrayPAT in a tracing experiment of ParaFEM/CGPACK MPI/coarray miniapp with cgca_gcupda.

Profiling with cgca_pfem_map



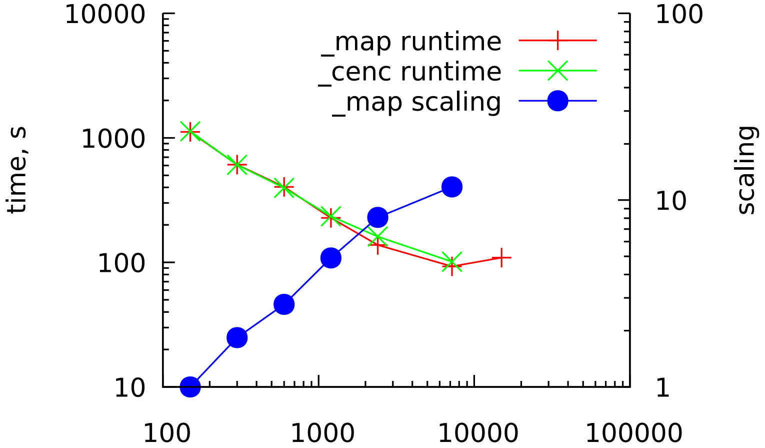
Profiling function distribution for ParaFEM/CGPACK MPI/coarray miniapp with cgca_gcupdn and cgca_pfem_map at 7200 cores.

Profiling with cgca_pfem_map

```
Table 1:  Profile by Function

  Samp% |    Samp |    Imb. |  Imb. |Group
        |         |    Samp | Samp% | Function
        |         |         |       |  PE=HIDE
        |         |         |       |   Thread=HIDE

 100.0% | 9,903.4 |      -- |    -- |Total
|-----------------------------------------------------------------
|  43.6% | 4,321.6 |      -- |    -- |USER
||----------------------------------------------------------------
||  31.4% | 3,110.7 |   589.3 | 15.9% |cgca_clvgp$cgca_m3clvg_
||   3.5% |   346.0 |   513.0 | 59.7% |cgca_hxi$cgca_m2hx_
||   3.5% |   342.0 |   175.0 | 33.8% |cgca_clvgn$cgca_m3clvg_
||   1.2% |   116.3 |     4.7 |  3.9% |cgca_pfem_map$cgca_m3pfem_
||   1.1% |   106.8 | 1,537.2 | 93.5% |cgca_clvgsd$cgca_m3clvg_
||   1.0% |    99.9 |    24.1 | 19.5% |cgca_sld$cgca_m3sld_
||================================================================
|  38.4% | 3,803.6 |      -- |    -- |MPI
||----------------------------------------------------------------
||  14.6% | 1,446.6 |   350.4 | 19.5% |mpi_bcast
||   9.4% |   932.4 |   473.6 | 33.7% |MPI_BARRIER
||   7.0% |   689.5 |   371.5 | 35.0% |mpi_recv
||   4.9% |   489.3 |    76.7 | 13.6% |MPI_ALLREDUCE
||   1.5% |   145.4 |   314.6 | 68.4% |MPI_REDUCE
||================================================================
|  17.8% | 1,766.8 |      -- |    -- |ETC
||----------------------------------------------------------------
||   9.9% |   983.9 |     8.1 |  0.8% |__DEALLOCATE
||   6.6% |   652.3 |    93.7 | 12.6% |gotoblas_dgemv_n_sandybridge
|=================================================================
```

Raw profiling data for ParaFEM/CGPACK MPI/coarray miniapp with cgca_gcupdn and cgca_pfem_map at 7200 cores.

Profiling with cgca_pfem_map



Runtimes and scaling for ParaFEM/CGPACK MPI/coarray miniapp with cgca_pfem_map and cgca_pfem_cenc.

cgca_pfem_map or cgca_pfem_cenc are called only once during the execution of the miniapp. Hence only a minor improvement is obtained, only from about 1000 cores.

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