Fortran coarray/MPI Multi-Scale CAFE for Fracture in Heterogeneous Materials

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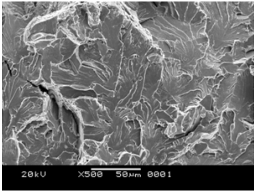
EPSRC Engineering and Physical Sciences Research Council

PARENG 2017, Pécs, Hungary 30th-31st May, 2017

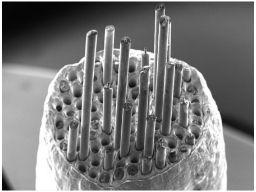
Fracture in heterogeneous materials



polycrystal cleavage

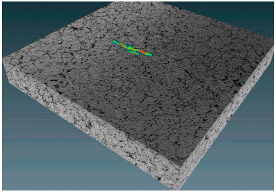
reinforced concrete

CFRP



metal matrix

bone

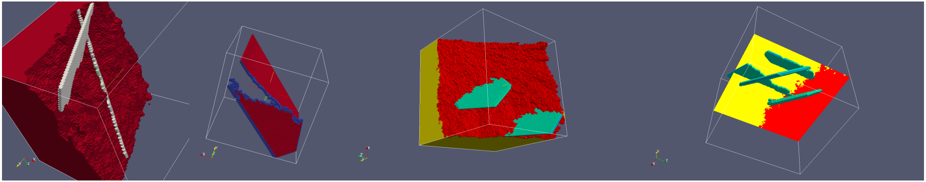


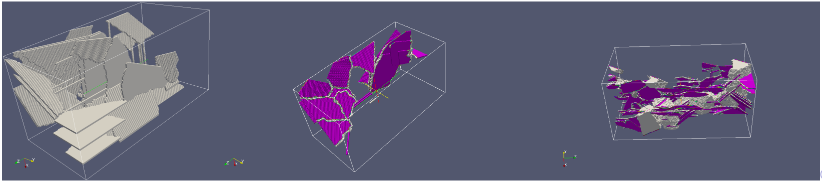
graphite

- All real materials are heterogeneous
- Multiple fracture and damage processes happen at different time and length scales $\rightarrow$ 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



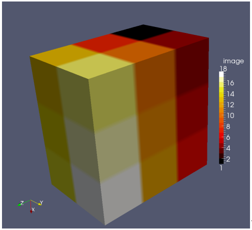


Fortran coarrays for CA

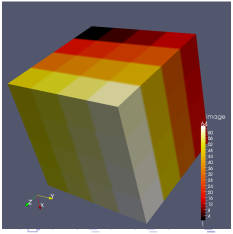
- Fortran native SPMD parallel programming feature
- Fortran standard since 2008. More features in 2015.
- Cray, Intel, OpenCoarrays/GCC support
- CGPACK - cellular automata microstructure simulation library: cgpack.sf.net. See also [1, 2, 3, 4].
- Easy halo exchange
- CA space coarray - 4D array, 3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

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

- Ideal for structured grids:

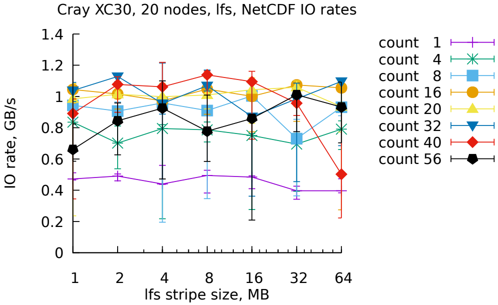


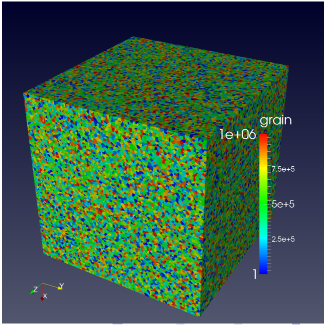
← 18 imgs; 64 imgs →



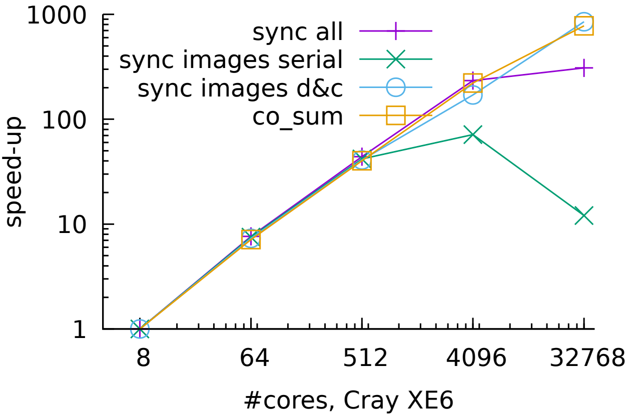
Coarray IO - no native Fortran parallel IO

- 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 [5])
- 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





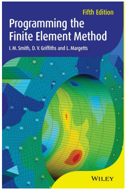
CGPACK solidification scaling

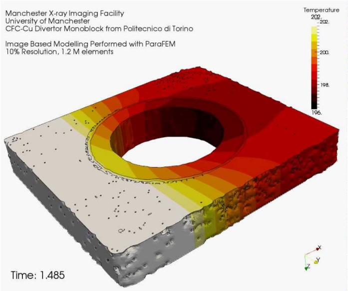


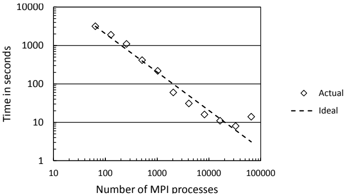
Scaling varies for different programs built with CGPACK, depending on which routines are called, in what order and requirements for synchronisation.

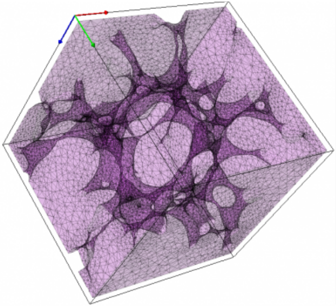
ParaFEM - scalable general purpose finite element library

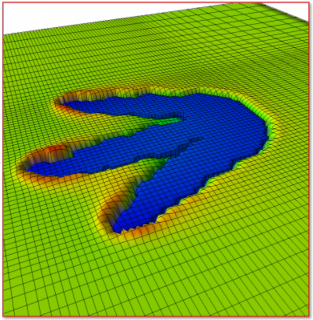
- http://parafem.org.uk
- Fortran 90 MPI
- Highly portable, many users [6]
- Excellent scaling
- BSD license



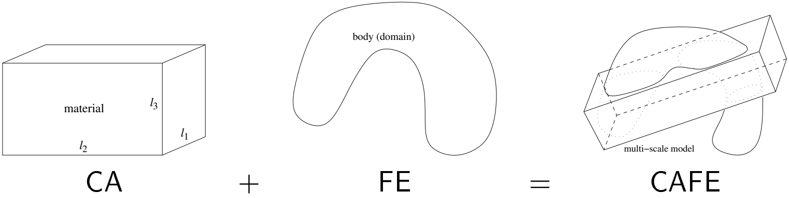


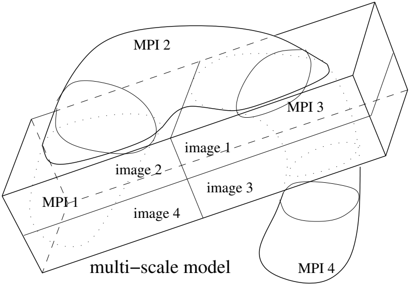


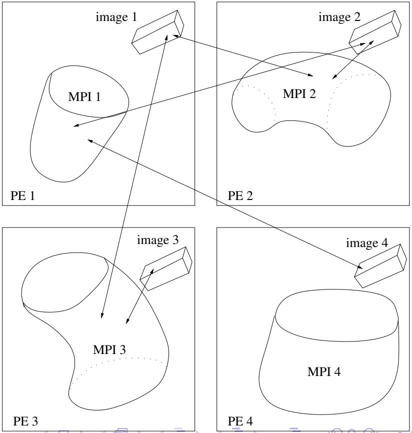




CAFE design: structured CA grid + unstructured FE grid

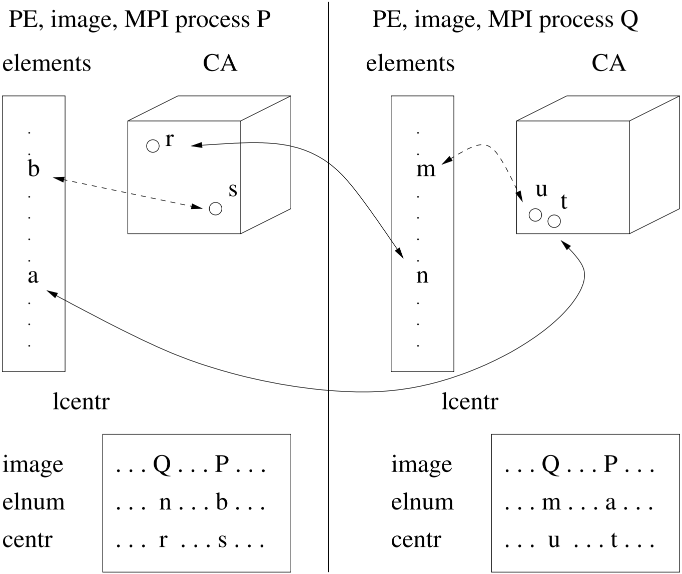






Example with 4 PE (4 MPI processes, 4 coarray images). Arrows are FE ↔ CA comms.

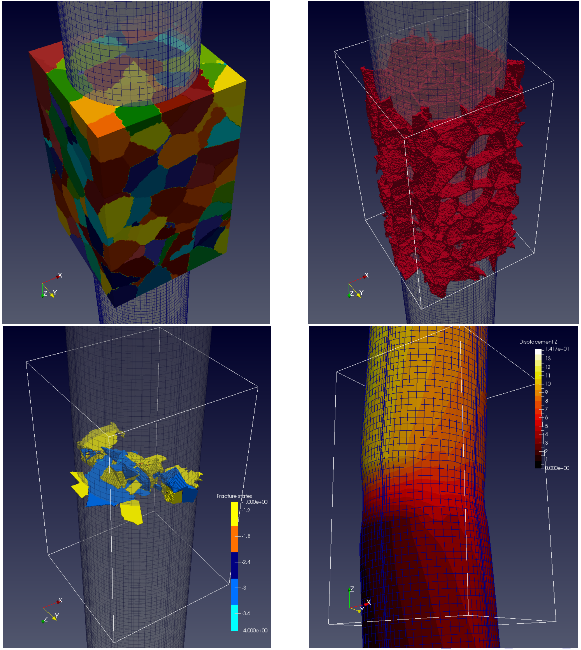
lcentr arrays on images P and Q



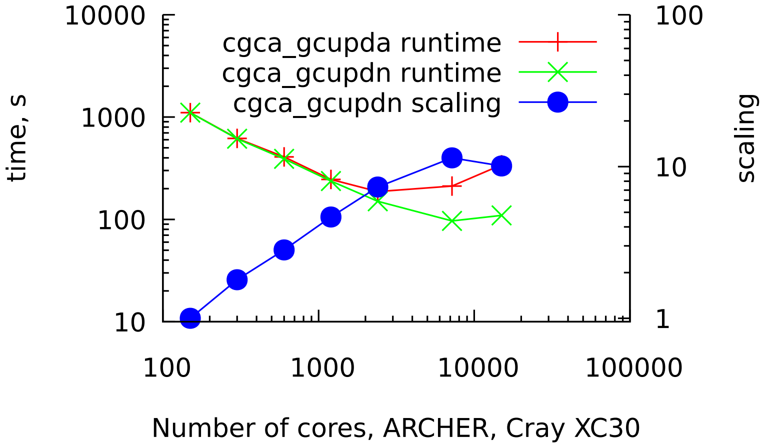
Fracture modelling

- 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} [2, 7].
- 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



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.

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 [8]

```
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 )
```

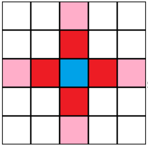
Conclusions

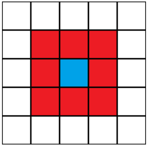
- Fortran coarrays are an ideal match for cellular automata
- Hybrid coarray+MPI multi-scale fracture framework is feasible
- Scaling up to 7k cores currently, work ongoing
- Profiling/tracing tools: CrayPAT, TAU, Score-P, Scalasca - coarray support is improving
- Coarray synchronisation - major issue: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

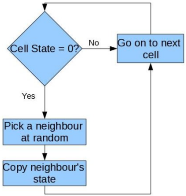
Cellular automata (CA) basics

- 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

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).



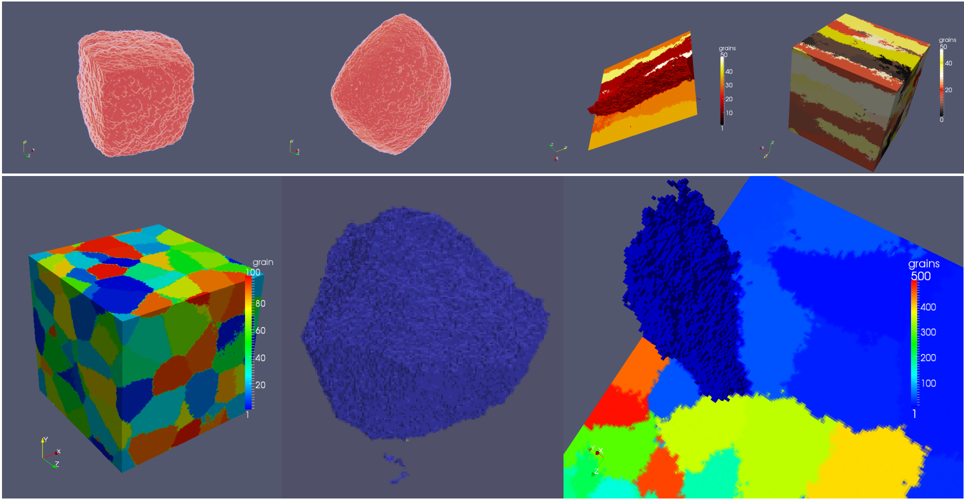
0	0	0	0	0	1	1	1	1
0	0	0	0	1	1	1	1	1
0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	24	24
0	0	0	0	0	24	1	24	24
0	0	0	0	0	24	24	24	24
0	0	0	0	24	24	24	24	24
0	0	0	24	24	24	24	24	24
0	0	24	24	24	24	24	24	24

i

0	0	0	1	1	1	1	1	1
0	0	0	0	1	1	1	1	1
0	0	0	1	1	1	1	1	1
0	0	0	0	24	1	1	24	24
0	0	0	0	0	24	1	24	24
0	0	0	0	0	24	24	24	24
0	0	0	24	24	24	24	24	24
0	0	24	24	24	24	24	24	24
0	0	24	24	24	24	24	24	24

$i + 1$

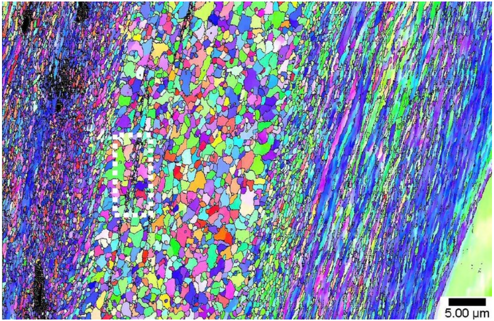
Primitive probabilistic 3D solidification - results

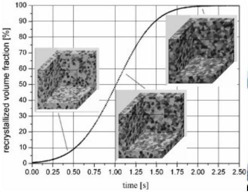


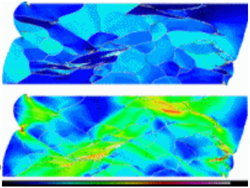
For more results ▸ CGPACK

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.

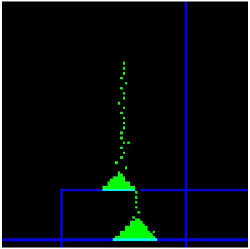




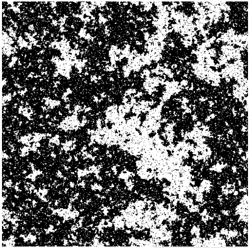


▸ Dierk Raabe site

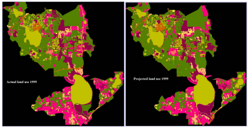
Other CA examples



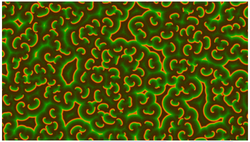
Sand pile formation



Ising magnetisation ▸ more info

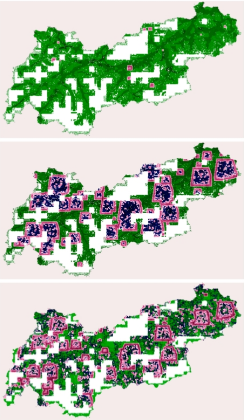


Land use ▸ more info



Diffusion ▸ animation ▸ info

Fire ▸ more info

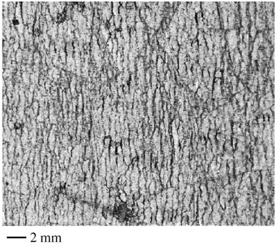


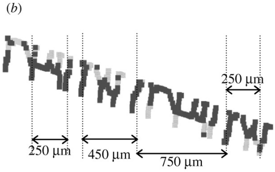
Epidemics, from The Open Med. Inform. J. 2(1):70-81, 2008.

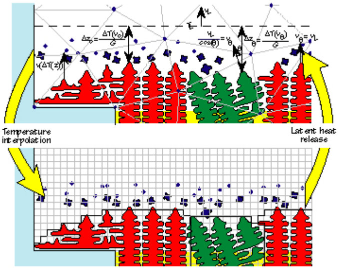
▸ PDF

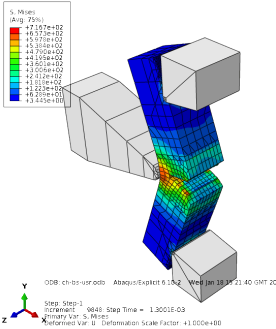
More CAFE examples

- Used for solidification [9], recrystallisation [10] and fracture [11, 12].
- FE - continuum mechanics - stress, strain, etc.
- CA - crystals, crystal boundaries, cleavage, grain boundary fracture
- FE → CA - stress, strain
- CA → FE - damage variables

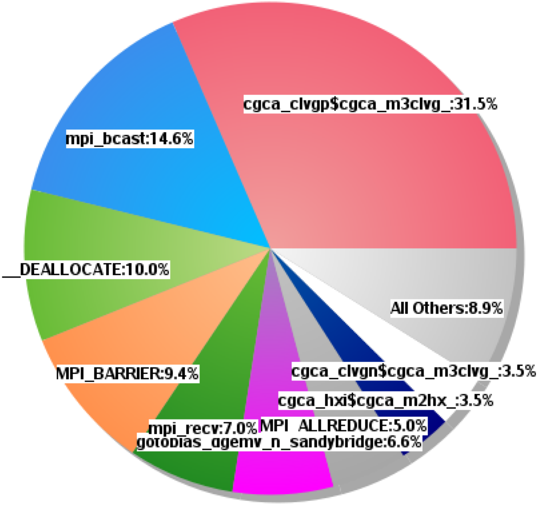








Profiling with cgca_pfem_map



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

Profiling with cgca_pfem_map

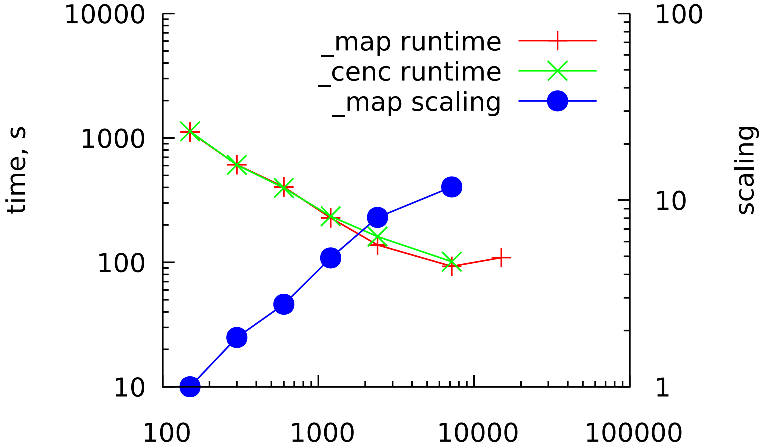
```
Table 1:  Profile by Function

  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.

[1] A. Shterenlikht, L. Margetts, and L. Cebamanos. Multi-scale CAFE framework for simulating fracture in heterogeneous materials implemented in fortran coarrays and mpi. In *PGAS Application Workshop (PAW), held in conjunction with SC16, Salt Lake City, UT, USA*, 2016. DOI: 10.1109/PAW.2016.006.

[2] A. Shterenlikht and L. Margetts. Three-dimensional cellular automata modelling of cleavage propagation across crystal boundaries in polycrystalline microstructures. *Proc. Roy. Soc. A*, 471:20150039, 2015.

[3] A. Shterenlikht, L. Margetts, L. Cebamanos, and D. Henty. Fortran 2008 coarrays. *ACM Fortran Forum*, 34:10–30, 2015.

[4] A. Shterenlikht. Fortran coarray library for 3D cellular automata microstructure simulation. In M. Weiland, A. Jackson, and N. Johnson, editors, *Proc. 7th PGAS Conf., 3-4 October 2013, Edinburgh, Scotland, UK*, pages 16–24. The University of Edinburgh, 2014.

[5] D. Henty, A. Jackson, C. Moulinec, and V. Szeremi. Performance of Parallel IO on ARCHER, version 1.1. ARCHER White Papers, 2015.

[6] I. M. Smith, D. V. Griffiths, and L. Margetts. *Programming the Finite Element Method*. Wiley, 5ed, 2014.

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