Fortran coarray library for 3D cellular automata microstructure simulation

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Outline

3D cellular automata models of materials

Fortran coarrays

Modelling results

Synchronisation, profiling and scaling

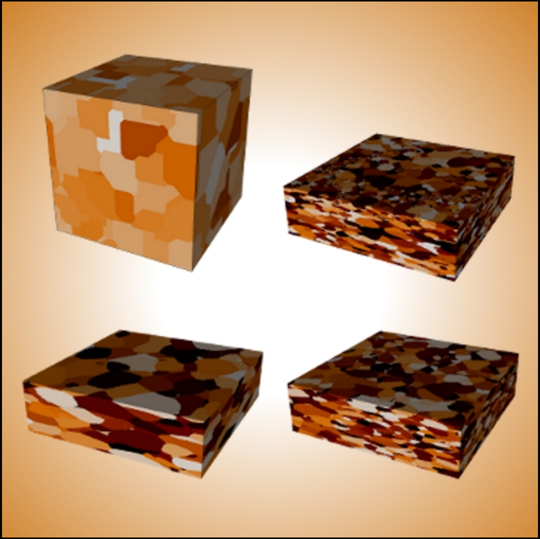
Unresolved: coarray I/O

Multiple physics, size and time scales

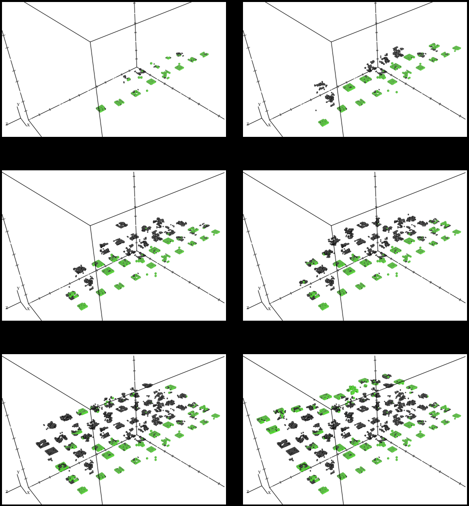
physics	size, m	time, s
recrystallisation	$10^{-9} \dots 10^{-2}$	$10^{-6} \dots 10^{5}$
cleavage	$10^{-6} \dots 10^{1}$	$10^{-6} \dots 10^{-3}$
ductile fracture	$10^{-8} \dots 10^{1}$	$10^{-6} \dots 10^{2}$
fatigue	$10^{-6} \dots 10^{-3}$	$10^{1} \dots \infty$
corrosion	?	?

- molecular dynamics
- discrete & continuous dislocation
- cellular automata, CA
- finite elements (boundary elements, meshless, etc.)

CA examples: recrystallisation

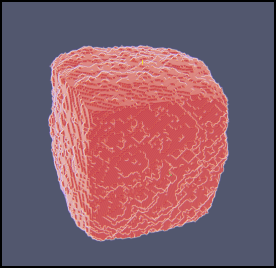


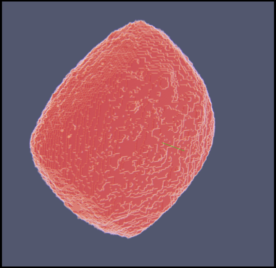
CA examples: ductile to brittle transitional fracture in steel – Charpy impact test [1]

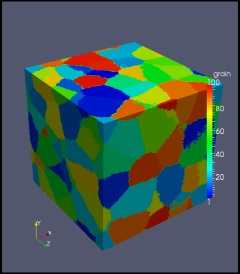


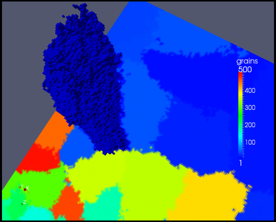
- Green - ductile failure
- Black - transgranular cleavage

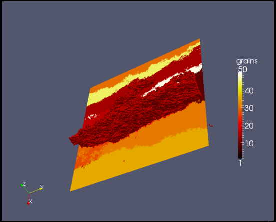
CA examples: single- and poly-crystals

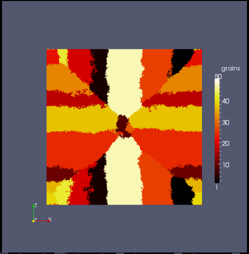




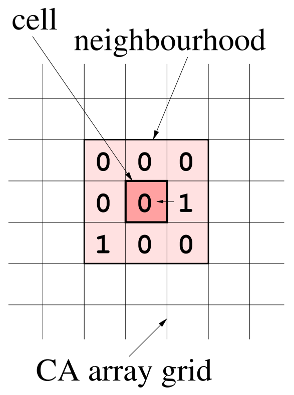








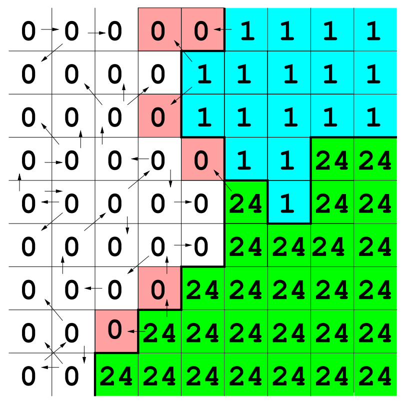
Basics of a 3D CA model



- 3D space, partitioned into identical cubic cells
- Self-similar or fixed boundaries
- Multiple, pre-defined cell states, e.g. liquid, grain, crack, etc.
- A grain is a collection of cells with the same state
- A neighbourhood of 26 nearest neighbours
- The state of each cell at $t+1$ is a function of the state of the neighbourhood at t

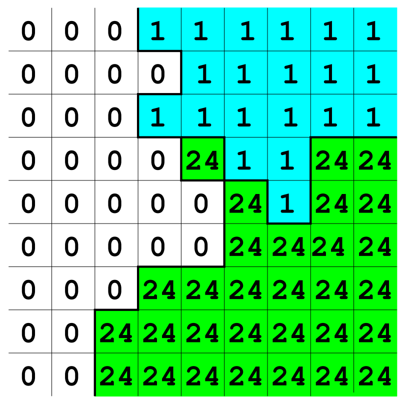
Basics of a 3D model: solidification

A liquid cell (state 0) acquires state of a randomly chosen neighbour:



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

t



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

$t+1$

CA computational challenge

- High spatial resolution is required, i.e. 10^5 cells per grain [2]
- Typical engineering steel has a grain size about $10^1 \ldots 10^2$ μm
- 1 cm^3 of such material might have $10^6 \ldots 10^9$ grains
- The model will need $10^{11} \ldots 10^{14}$ cells
- A complete solution might require $10^3 \ldots 10^5$ iterations

Conclusion: need lots of memory and fast processing!

Fortran coarray basics

- Simple new syntax for SIMD problems
- Feature of Fortran 2008 standard [3]
- Fortran coarrays, **NOT** Coarray fortran or CAF
- Standard Fortran is important for linking with other Fortran codes
- Coarray collectives and teams by about 2015 [4]
- Cray provide collectives as an extension to the standard
- Cray and Intel coarray support is most comprehensive [5]
- Most thoroughly explained in "MFE" – Metcalf, Reid, Cohen (2011) Modern Fortran Explained [6]

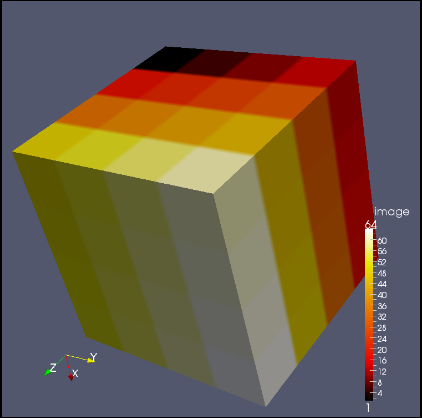
Fortran coarray example

```
integer :: i[*]                        ! scalar coarray
real,allocatable :: r(:)[:]            ! array coarray
integer :: img, num
img = this_image()                     ! new f2008 intrinsic
num = num_images()                     ! new f2008 intrinsic
i = img
r = 1.0
allocate (r(100)[*])                   ! allocating array coarray
if (img .eq. 1   ) &
 i = i + i[num]                        ! remote read
if (img .eq. num) &
 r(5)[1] = sum(r)                      ! remote write
end
```

CA data structures

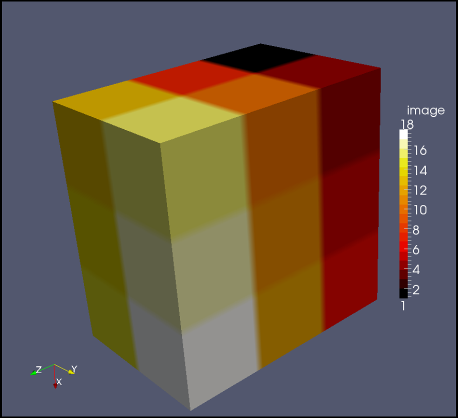
- Model *assembly*, not *partition*: `real :: z(1000)[*]` run on 64 images effectively gives a real array of 64,000
- Coarrays waste memory, use sparingly
- The model itself:
  `integer,allocatable :: coarray(:,:,:,:)[:,:,:]`
  note 3D image grid, to minimise boundary area, i.e. minimise halo exchange data transfer
- Various other arrays, depending on the need, e.g. the grain size:
  `integer,allocatable :: gs(:)[:,:,:]`
  note the wasted memory

CA model coarray



```
allocate( &
coarray(10,10,10)[4,4,*])
```

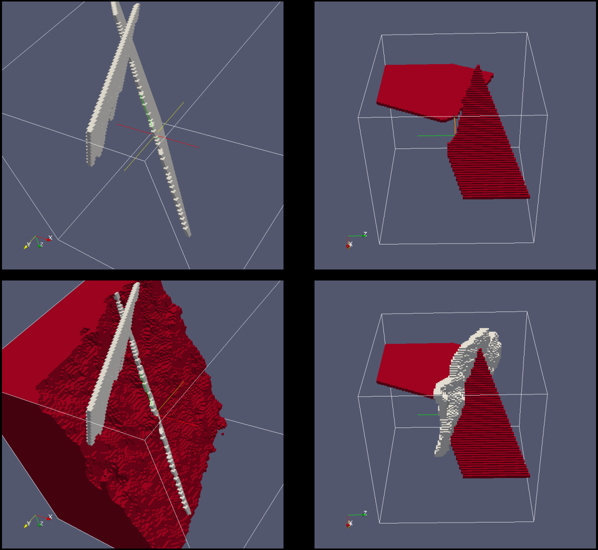
on 64 images



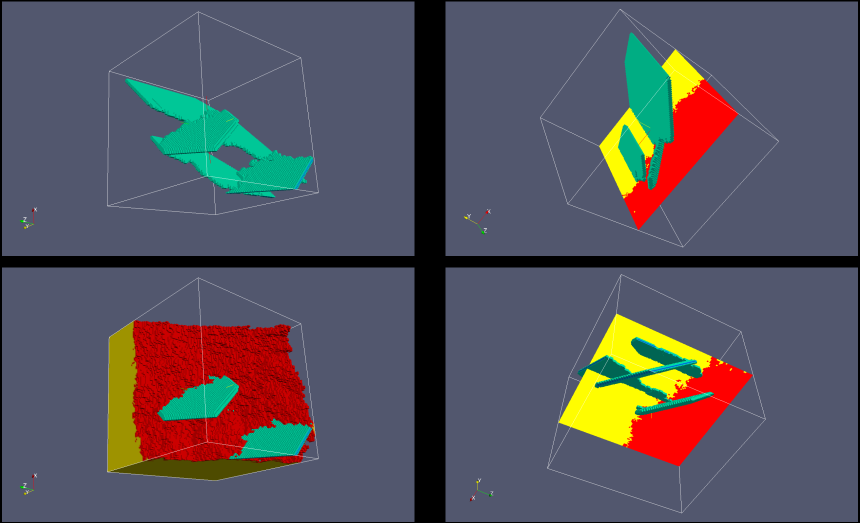
```
allocate( &
coarray(10,10,10)[3,2,*])
```

on 18 images

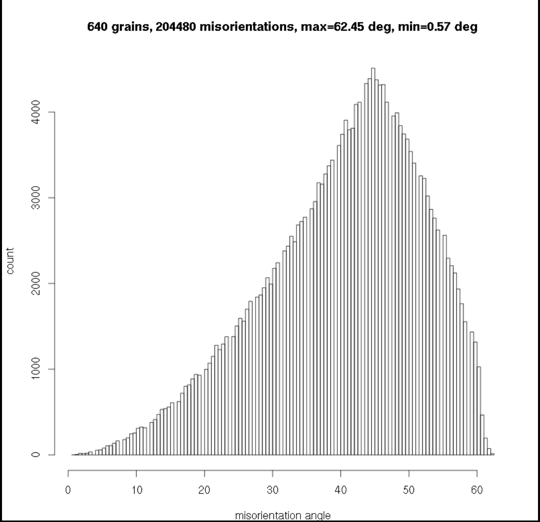
Modelling results: cleavage 1



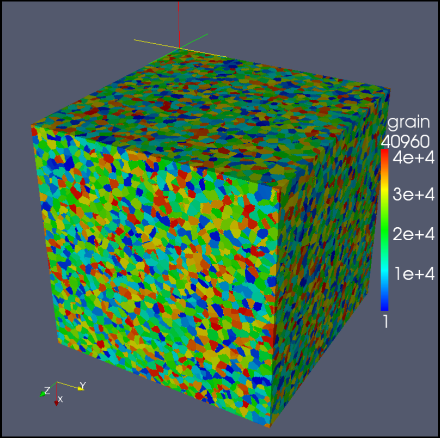
Modelling results: cleavage 2

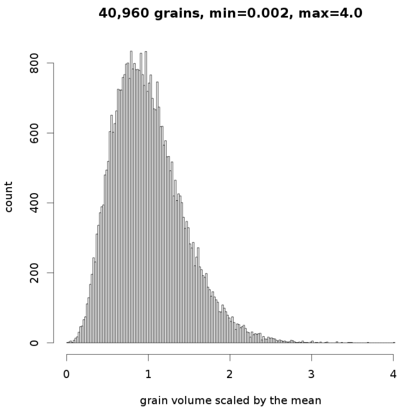


Modelling results: grain mis-orientation distribution



Modelling results: micro-structure, 10^9 cells





Solidification kernel

```
integer :: fin, x1, x2, x3, z(3), lbr(3), ubr(3)
logical :: finished
real :: candidate(3)
main: do
  array = space( :, :, :, type_grain )
  do x3 = lbr(3),ubr(3)
  do x2 = lbr(2),ubr(2)
  do x1 = lbr(1),ubr(1)
    if ( space( x1, x2, x3, type_grain ) .eq. liquid ) then
      call random_number( candidate )     ! 0 .le. candidate .lt. 1
      z = nint( candidate*2 - 1 )         ! step = [-1 0 1]
      array( x1,x2,x3 ) = space( x1+z(1), x2+z(2), x3+z(3), type_grain )
    end if
  end do
  end do
  end do
  space( :, :, :, type_grain ) = array
  finished = all( space( lbr(1):ubr(1), lbr(2):ubr(2), lbr(3):ubr(3), &
                   type_grain ) .ne. liquid )
  fin = 1                   ! not solid yet
  if (finished) fin = 0     ! solid
!!!  exit if (fin .eq. 0) on *all* images
end do main
```

Synchronising solidification

```
integer :: fin, x1, x2, x3, z(3), lbr(3), ubr(3)
logical :: finished
real :: candidate(3)
main: do

call hxi(coarray) ! halo exchange - remote read only - no sync required!

! kernel

  finished = all( space( lbr(1):ubr(1), lbr(2):ubr(2), lbr(3):ubr(3), &
                   type_grain ) .ne. liquid )
  fin = 1                   ! not solid yet
  if (finished) fin = 0     ! solid

! some sync required
! global reduction
! some sync required

!!!  exit if (fin .eq. 0) on *all* images

end do main
```

Global reduction

1. Image 1 does all reduction work, other images wait
2. All images do reduction work, one at a time
3. Divide & conquer
4. Cray collectives

In the following:

```
  img = this_image()
nimgs = num_images()
```

Global reduction: serial algorithms

image 1 only

```
if ( img .eq. 1 ) then
  do i = 2,nimgs
    fin = fin + fin[i]
  end do
end if

sync all
fin = fin[1]
```

all images in turn

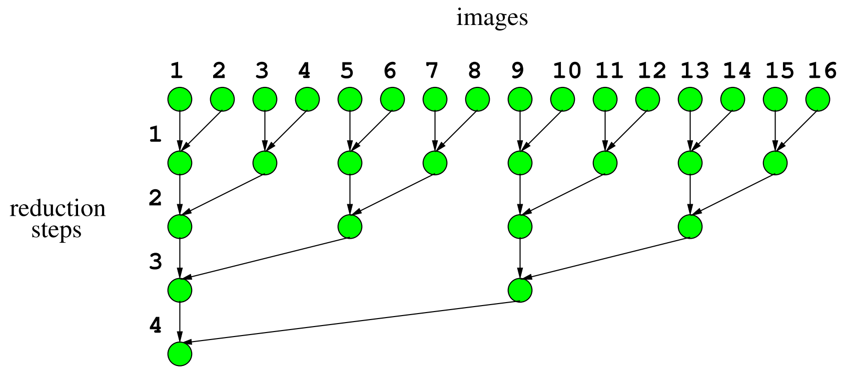
```
if ( img .ne. 1 ) then
  sync images (img - 1)
  fin[1] = fin[1] + fin
end if

if ( img .lt. nimgs )&
  sync images (img + 1)

sync all
fin = fin[1]
```

On `sync images`

- `sync images` are *not* tagged!
- `sync images` must match!
  From the standard [3]:

  > *Executions of SYNC IMAGES statements on images M and T correspond if the number of times image M has executed a SYNC IMAGES statement with T in its image set is the same as the number of times image T has executed a SYNC IMAGES statement with M in its image set.*

Divide & conquer or a binary tree



2^p images need p reduction steps.
Generally n images need $\log n$ steps.

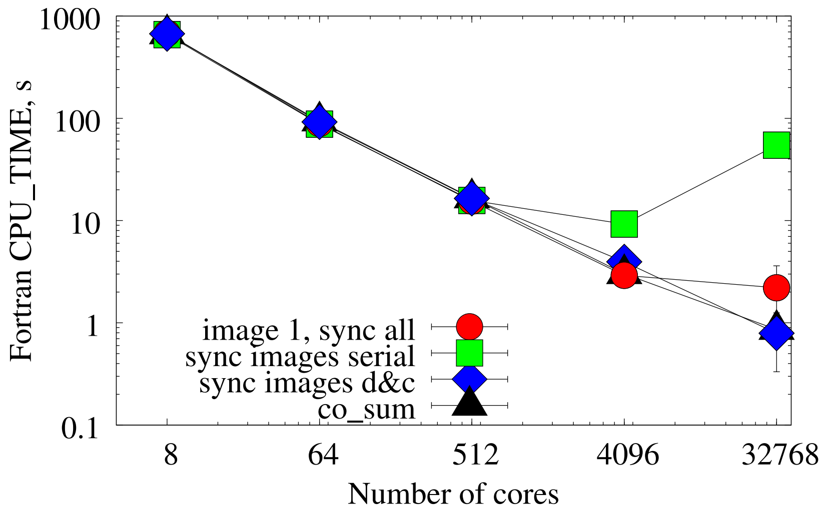
Divide & conquer synchronisation

```
step    = 2
stepold = 1
redu: do i = 1,p
  if ( mod(img,step) - 1 .eq. 0 ) then
    sync images ( img + stepold )
    fin = fin + fin[ img + stepold ]
  else if ( mod(img+stepold,step) - 1 .eq. 0 ) then
    sync images ( img - stepold )
  end if
  stepold = step
  step = step * 2
end do redu

sync all
fin = fin[1]
```

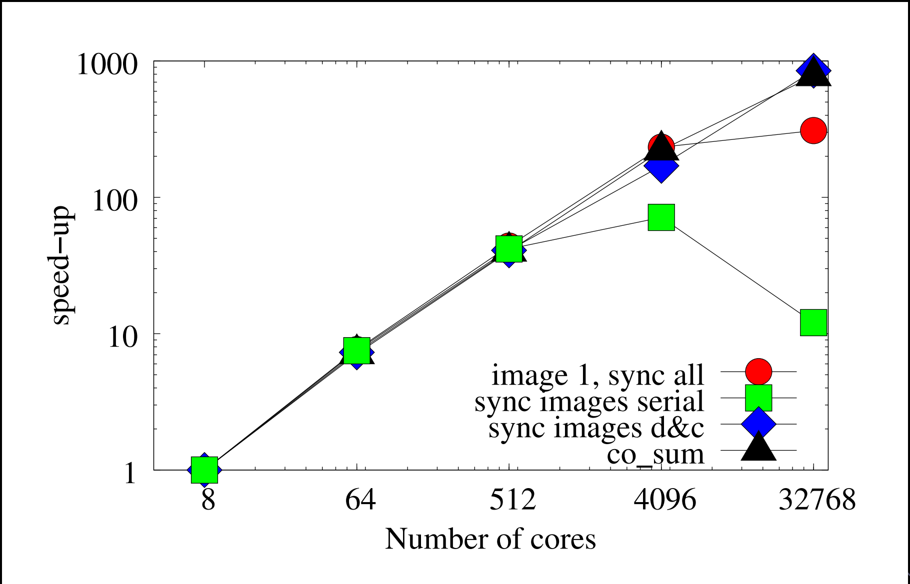
Cray `co_sum` reduction

- Cray extension to the standard [3]
- Quite similar to what is proposed in TS 18508 [4]
- Must be called by all images
- Can be used 'only in a context that allows an image control statement' [4]
- Hence synchronisation might or might not be required, depending on the algorithm
- No synchronisation is required in the solidification algorithm!
- `call co_sum(fin)`

Performance : HECToR XE6 : time



Performance : HECToR XE6 : speedup



Performance : HECToR XE6 : conclusion

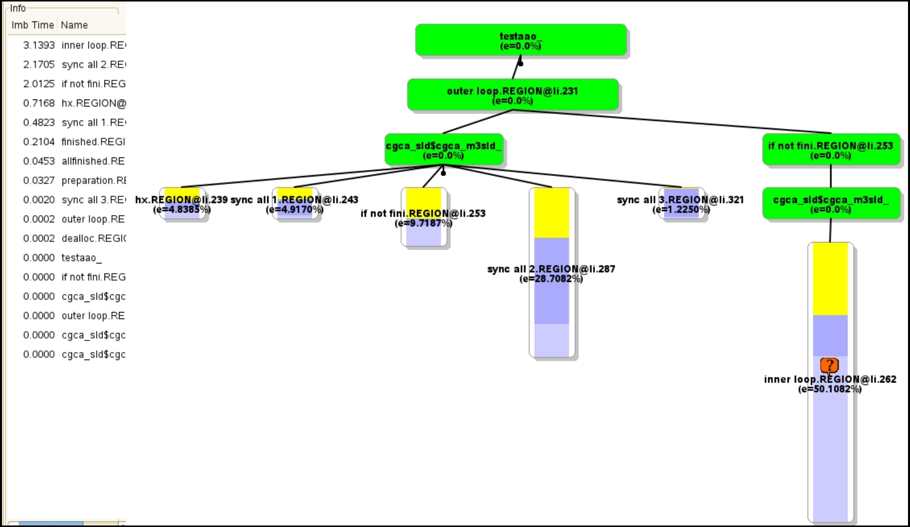
- A model with 2^{30} cells
- From $2^3 = 8$ cores, as: `coarray(512,512,512)[2,2,2]`
- to $2^{15} = 32768$ cores as: `coarray(32,32,32)[32,32,32]`
- The times calculated with `cpu_time` intrinsic
- The speed-up is nearly 10^3 for the core count raising by a factor of $2^{12} = 4096$!

Profiling: CrayPAT [7] on HECToR XE6

- API calls

-
  ```
  call pat_region_begin(num, "name", pat_status)
  ...
  call pat_region_end  (num,         pat_status)
  ```
- Profiling runs were done on 4096 processors

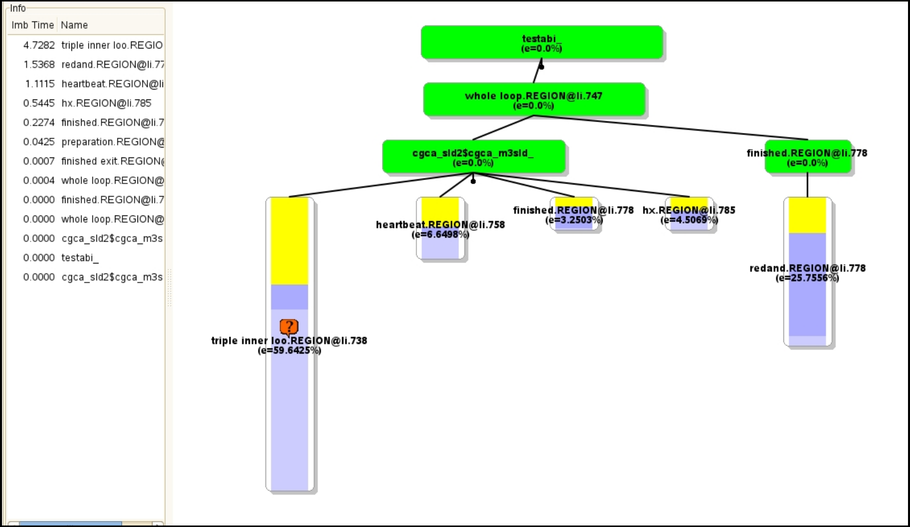
Profiling: serial reduction



Info

Imb Time	Name
3.1393	inner loop.RE
2.1705	sync all 2.RE
2.0125	if not fini.REG
0.7168	hx.REGION@
0.4823	sync all 1.RE
0.2104	finished.REGI
0.0453	allfinished.RE
0.0327	preparation.RE
0.0020	sync all 3.RE
0.0002	outer loop.RE
0.0002	dealloc.REGI
0.0000	testaao_
0.0000	if not fini.REG
0.0000	cgca_sld$cgc
0.0000	outer loop.RE
0.0000	cgca_sld$cgc
0.0000	cgca_sld$cgc

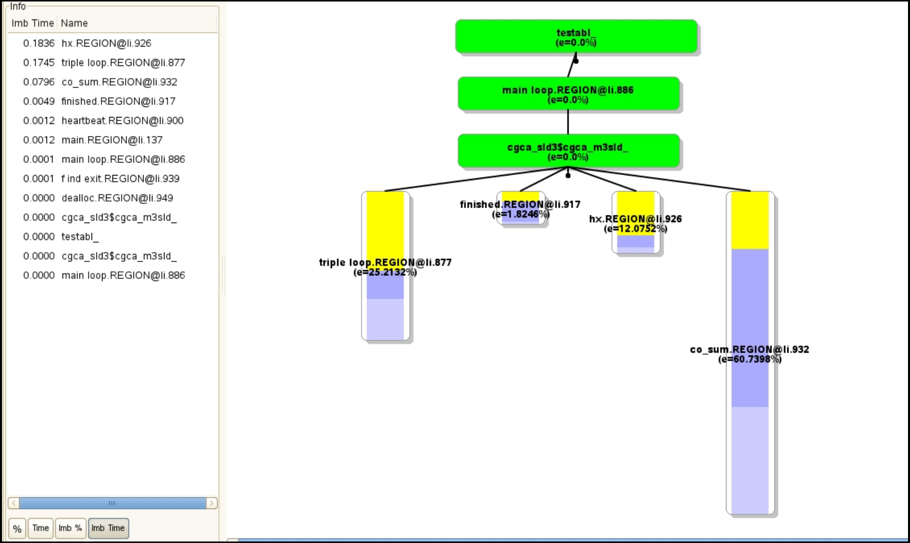
Profiling: divide & conquer reduction



Info

Imb Time	Name
4.7282	triple inner loo.REGIO
1.5368	redand.REGION@li.77
1.1115	heartbeat.REGION@li
0.5445	hx.REGION@li.785
0.2274	finished.REGION@li.7
0.0425	preparation.REGION@
0.0007	finished exit.REGION(
0.0004	whole loop.REGION@
0.0000	finished.REGION@li.7
0.0000	whole loop.REGION@
0.0000	cgca_sld2$cgca_m3s
0.0000	testabi_
0.0000	cgca_sld2$cgca_m3s

Profiling: Cray collective `co_sum` reduction



Info

Imb Time	Name
0.1836	hx.REGION@li.926
0.1745	triple loop.REGION@li.877
0.0796	co_sum.REGION@li.932
0.0049	finished.REGION@li.917
0.0012	heartbeat.REGION@li.900
0.0012	main.REGION@li.137
0.0001	main loop.REGION@li.886
0.0001	f ind exit.REGION@li.939
0.0000	dealloc.REGION@li.949
0.0000	cgca_sld3$cgca_m3sld_
0.0000	testabl_
0.0000	cgca_sld3$cgca_m3sld_
0.0000	main loop.REGION@li.886

Profiling: conclusion

Relative times, %, spent in different parts of the solidification routines and the total run time in seconds.

	`sync all`	d&c	`co_sum`
triple loop	50	60	25
global reduction	35	25	61
serial reduction + I/O	10	10	2
halo exchange	5	5	12
Time, s	35	47	20

- `co_sum` spends twice as long doing the global reduction as the triple loop computation
- With image 1 + `sync all` and with divide & conquer the triple loop takes roughly twice as long as the global reduction.
- `co_sum` approach is twice as fast overall

Coarray I/O

- From [6]:

> *Although a file is not permitted to be connected to more than one image in Fortran 2008, it is expected that a forthcoming Technical Report will define such a facility.*

- The first part is true
- The second part is not so true anymore [4]!
- Multiple writers, multiple files – tried, bad
- Single writer, single file - tried, more on this later
- Multiple writers, single file - not supported
- Few writers, few files - not tried, possibly using MPI-IO

Coarray I/O: single writer, single file

```
if (this_image() .eq. 1) then
    open(unit=iounit, file=fname, access="stream", &
         form = "unformatted", status = "replace")
do coi3 = lcob(3), ucob(3)                     !  Nested loops
  do i3 = lb(3), ub(3)                         !  for writing
    do coi2 = lcob(2), ucob(2)                 !  in correct order
      do i2 = lb(2), ub(2)                     !  from all images.
        do coi1 = lcob(1), ucob(1)             !
          write( unit = iounit )    &          !  Write one column
            coarray(lb(1):ub(1),i2,i3) &       !  at a time
            [coi1, coi2, coi3]                 !  Don't write halos!
          end do
        end do
      end do
    end do
  end do
end if
```

Simple, but extremely expensive!

Further development of the library

- Linking with a parallel FE library - possibly ParaFEM [8] - a CAFE model
- Optimising I/O
- Exploring OpenMP + coarrays for speeding up nested loops
- Looking for good PhD candidates in: metallurgy, physics, numerical methods, HPC, visualisation, etc.
- Freely available under BSD license from http://eis.bris.ac.uk/∼mexas/cgpack

Conclusions

- Fortran coarrays - simple, but flexible and powerful!
- Fortran coarray data structures are recommended for CA modelling.
- Speed-up of 10^3 from 8 to 30k cores was achieved.
- Optimising synchronisation and minimising single image computation are the key to good performance.

Acknowledgments

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- David Henty (EPCC) for the Fortran coarray course
- Reinhold Bader (LRZ) for the Advanced Fortran course
- Reviewers for helpful suggestions!

References

[1] A. Shterenlikht and I. C. Howard. The CAFE model of fracture – application to a TMCR steel. *Fatigue and Fracture of Engineering Materials and Structures*, 29:770–787, 2006.

[2] J. Phillips, A. Shterenlikht, and M. J. Pavier. Cellular automata modelling of nano-crystalline instability. In *Proceedings of the 20th UK Conference of the Association for Computational Mechanics in Engineering, 27-28 March 2012, The University of Manchester, UK*, 2012.

[3] ISO/IEC 1539-1:2010. *Fortran – Part 1: Base language, International Standard*. 2010. http://j3-fortran.org/doc/standing/links/007.pdf.

[4] ISO/IEC JTC1/SC22/WG5 N1983. *Additional Parallel Features in Fortran*. JUL-2013. ftp://ftp.nag.co.uk/sc22wg5/N1951-N2000/N1983.pdf.

[5] I. D. Chivers and J. Sleightholme. Compiler support for the fortran 2003 and 2008 standards, revision 12. *ACM Fortran Forum*, 32(1):8–19, 2013. www.fortranplus.co.uk/resources/fortran_2003_2008_compiler_support.pdf.

[6] M. Metcalf, J. Reid, and M. Cohen. *Modern Fortran explained*. Oxford University Press, 7 edition, 2011.

[7] Cray Inc. *Using Cray Performance Measurement and Analysis Tools*. MAR-2013. http://docs.cray.com/books/S-2376-610/.

[8] ParaFEM - A General Parallel Finite Element Message Passing Library, Research Computing Services, The University of Manchester, UK, 2009. http://www.parafem.org.uk/ (HTML).