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User Experiments with PGAS Languages, or

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Will Sawyer, Sergei Isakov, Adrian Tineo

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  - MPI + OpenMP hybrid programming
  - MPI-2 one-sided communication
  - SHMEM
  - PGAS languages (CAF, UPC)
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- Compare performance across platforms
  - out-of-the-box performance
  - evaluate optimization effort
  - socket-for-socket, node-for-node, energy-to-solution comparisons

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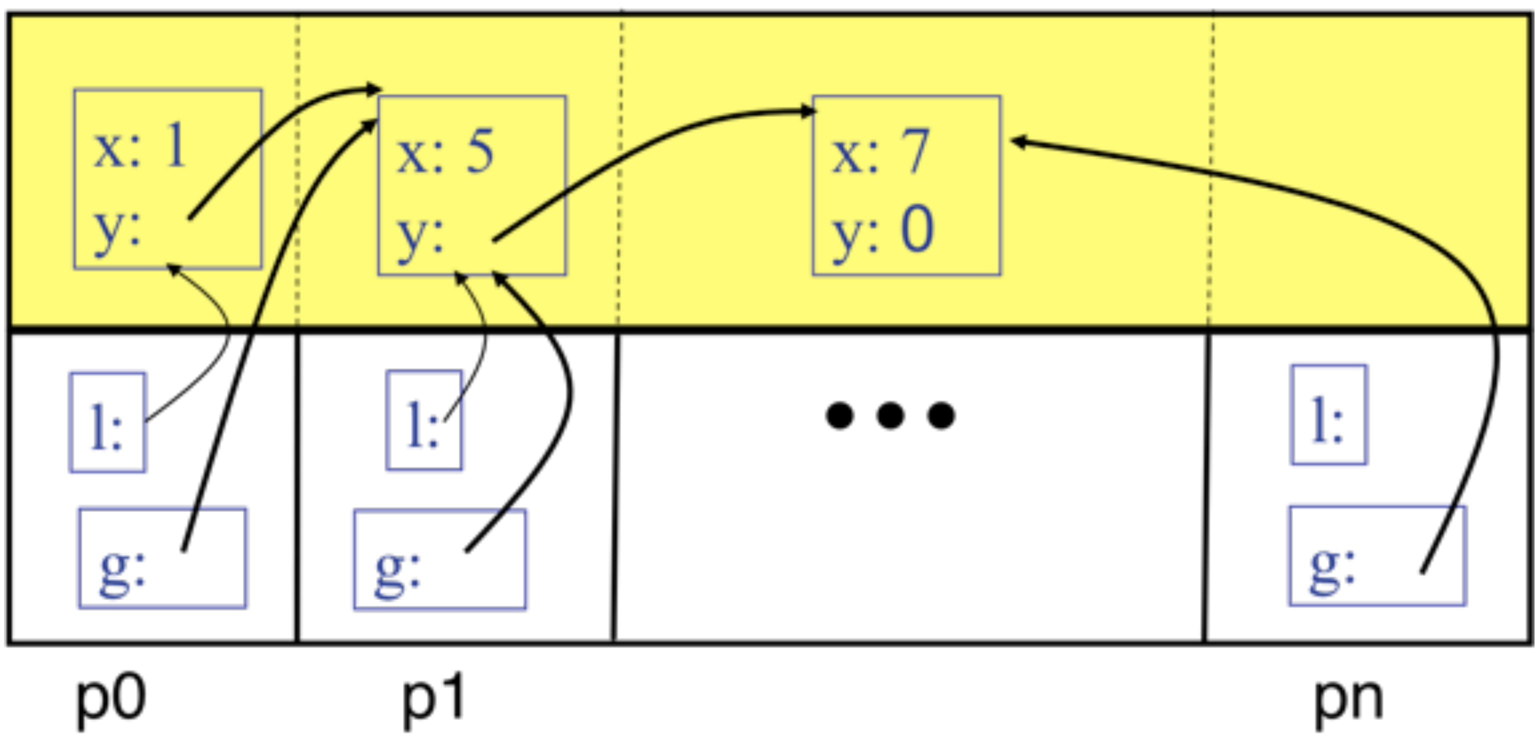

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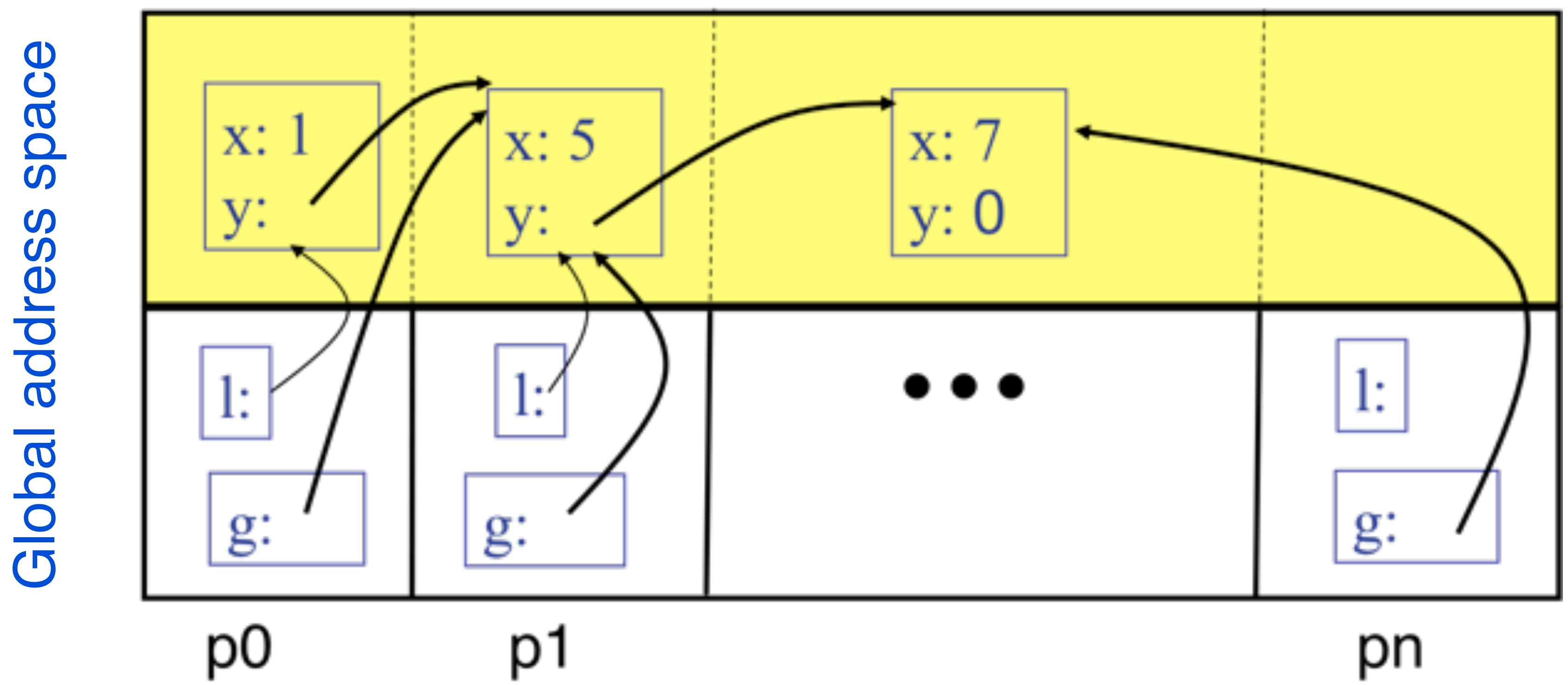

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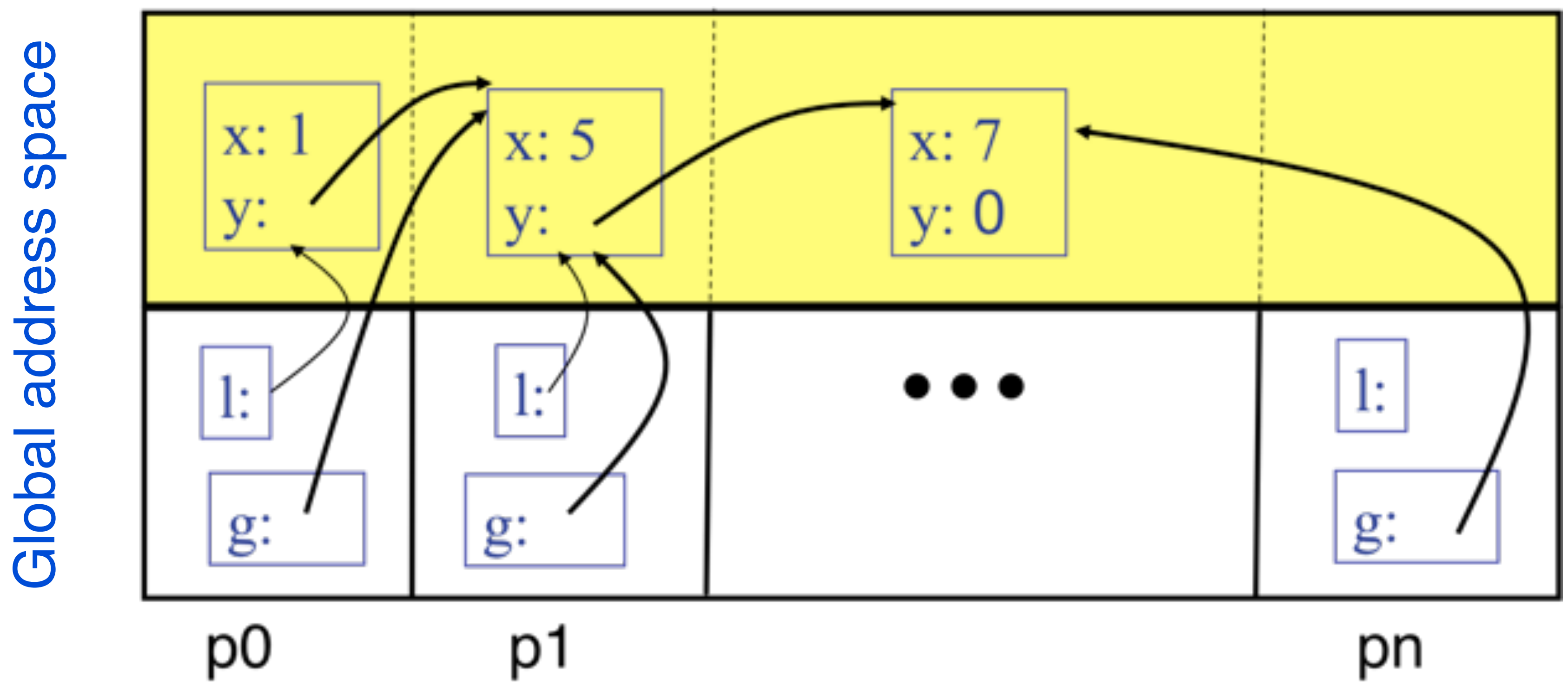

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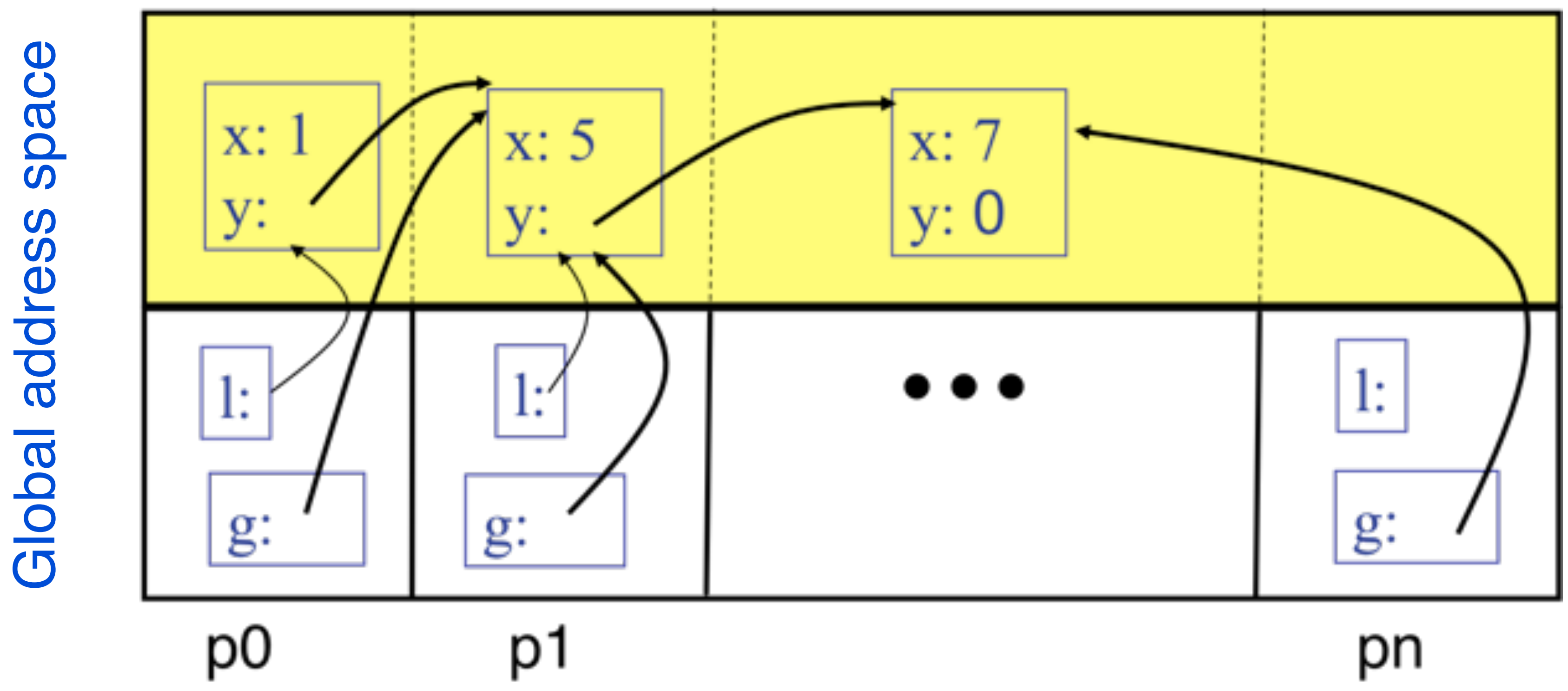

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3 Current languages: UPC, CAF, and Titanium

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- Potential interoperability with existing C/Fortran/Java code

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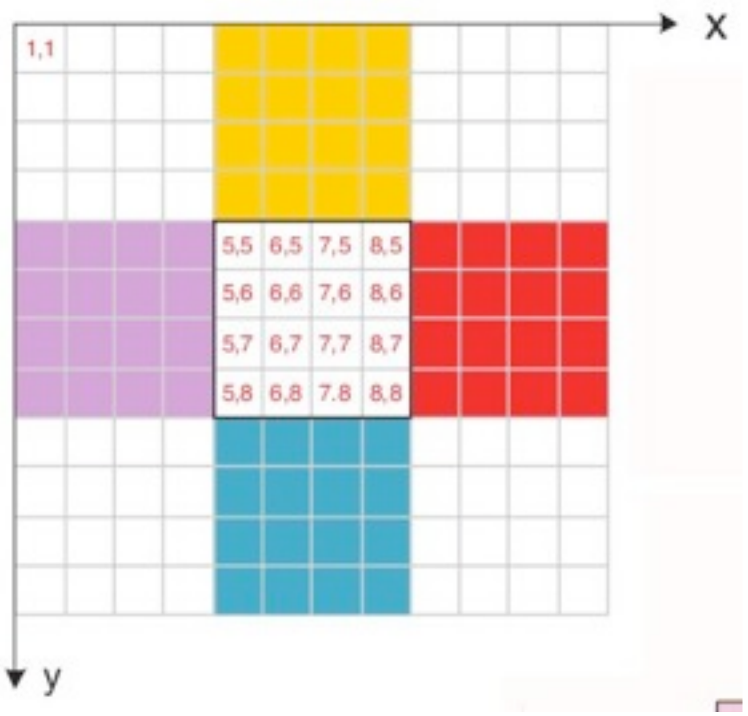

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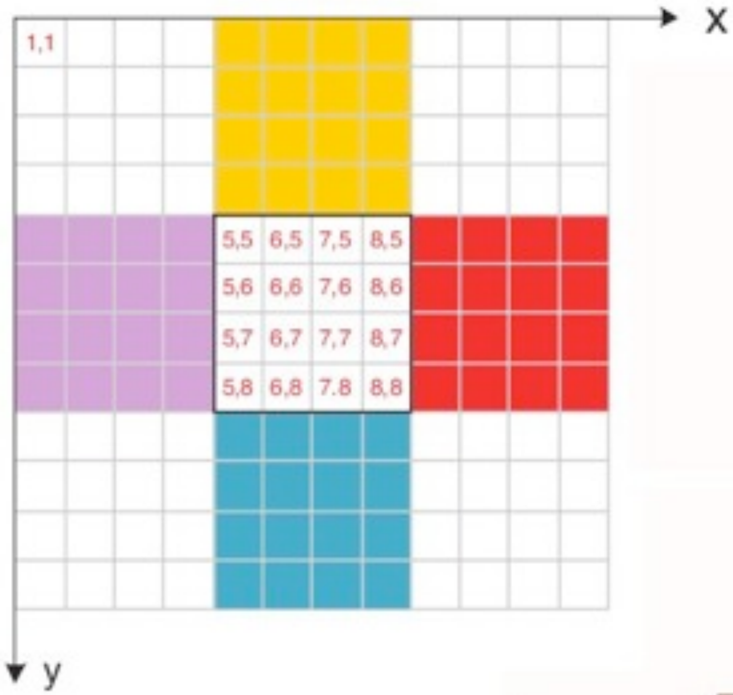

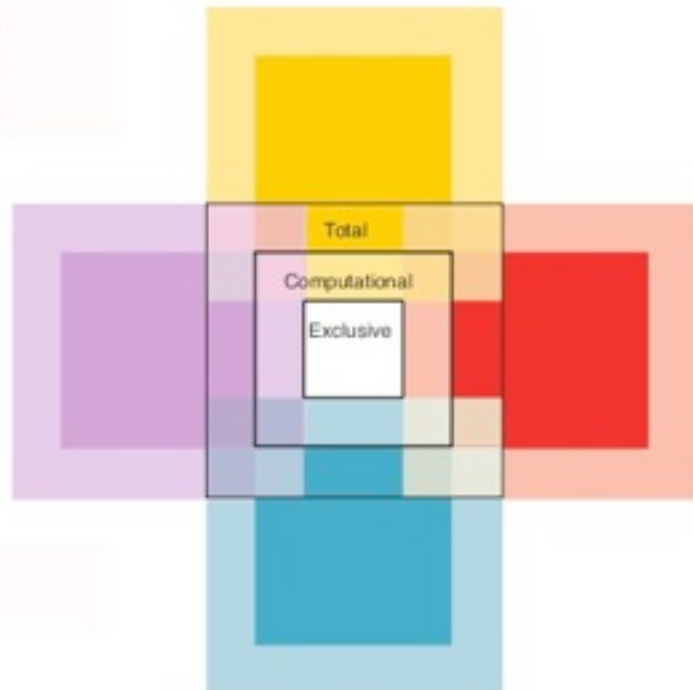

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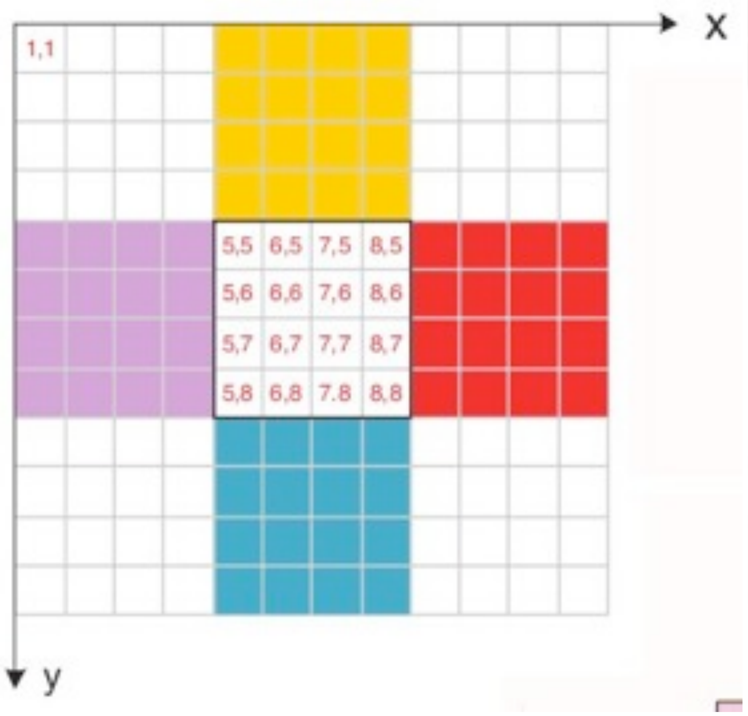

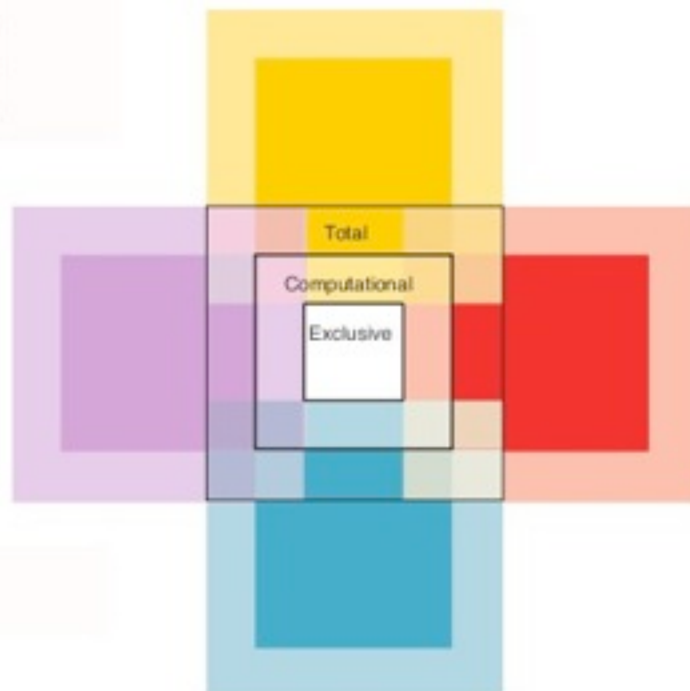

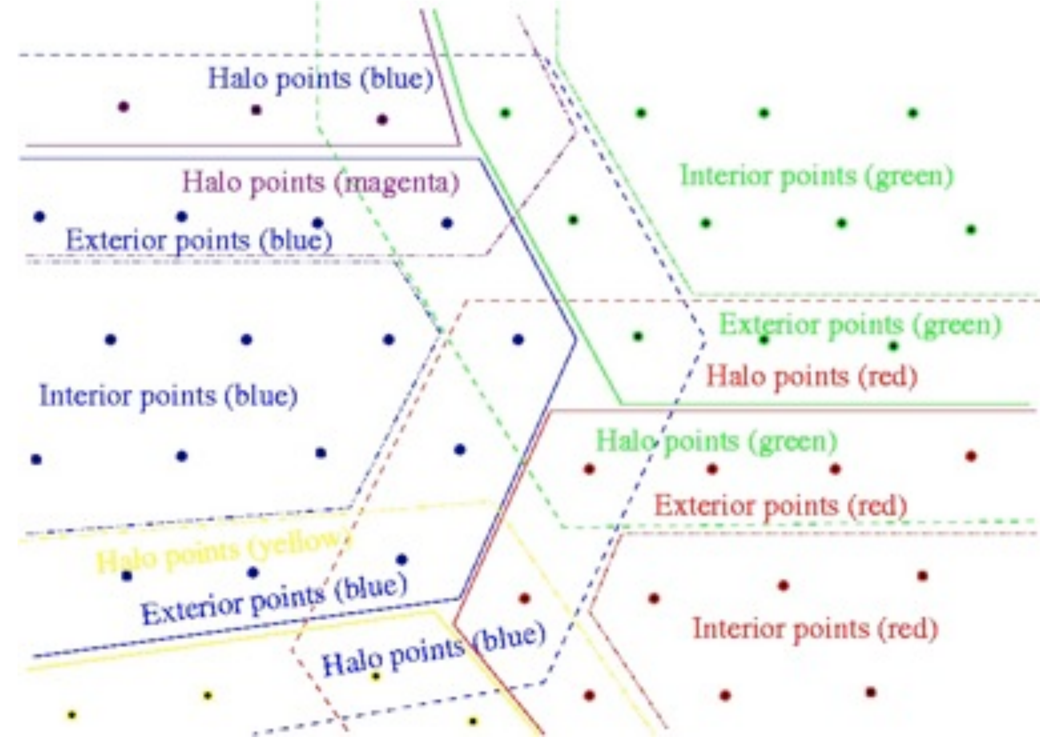

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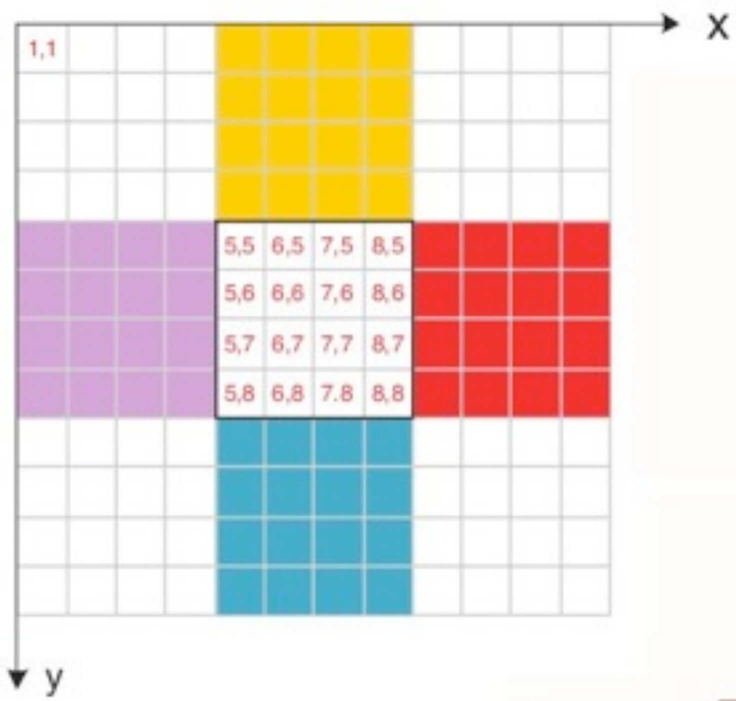

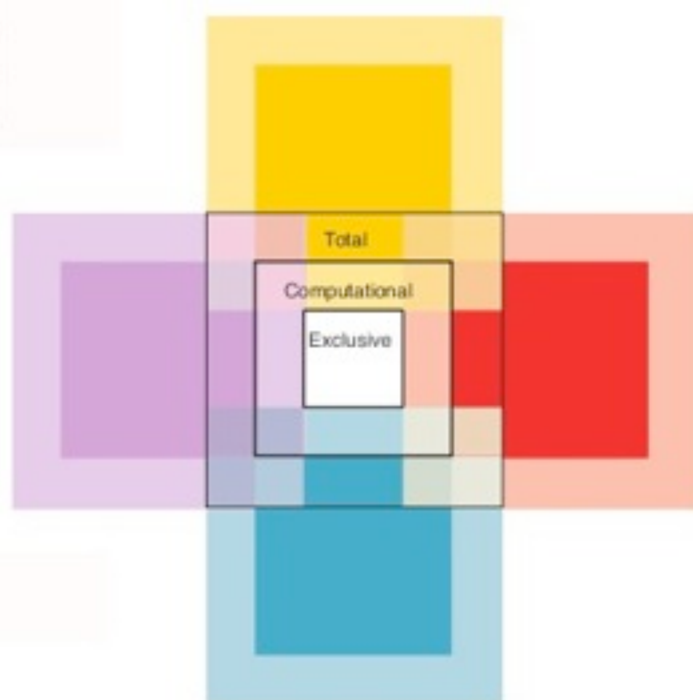

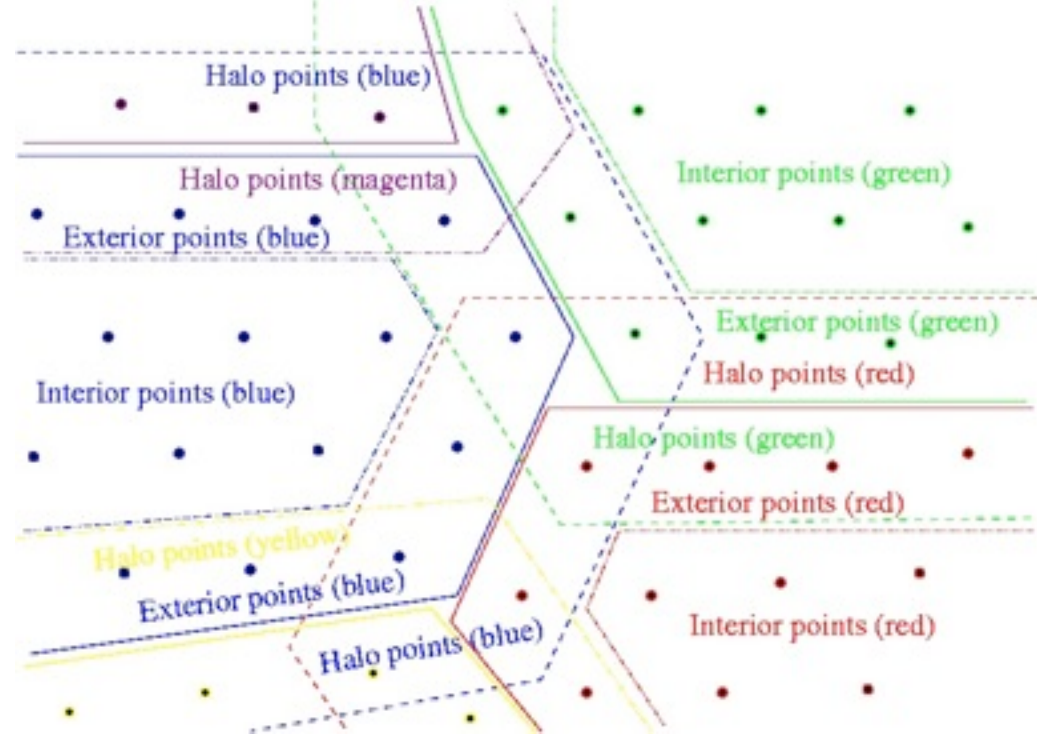

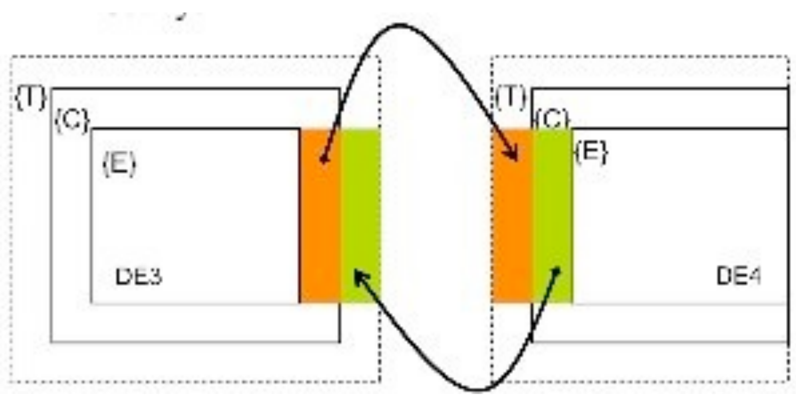

Potential Performance Gains with Co-Array Fortran

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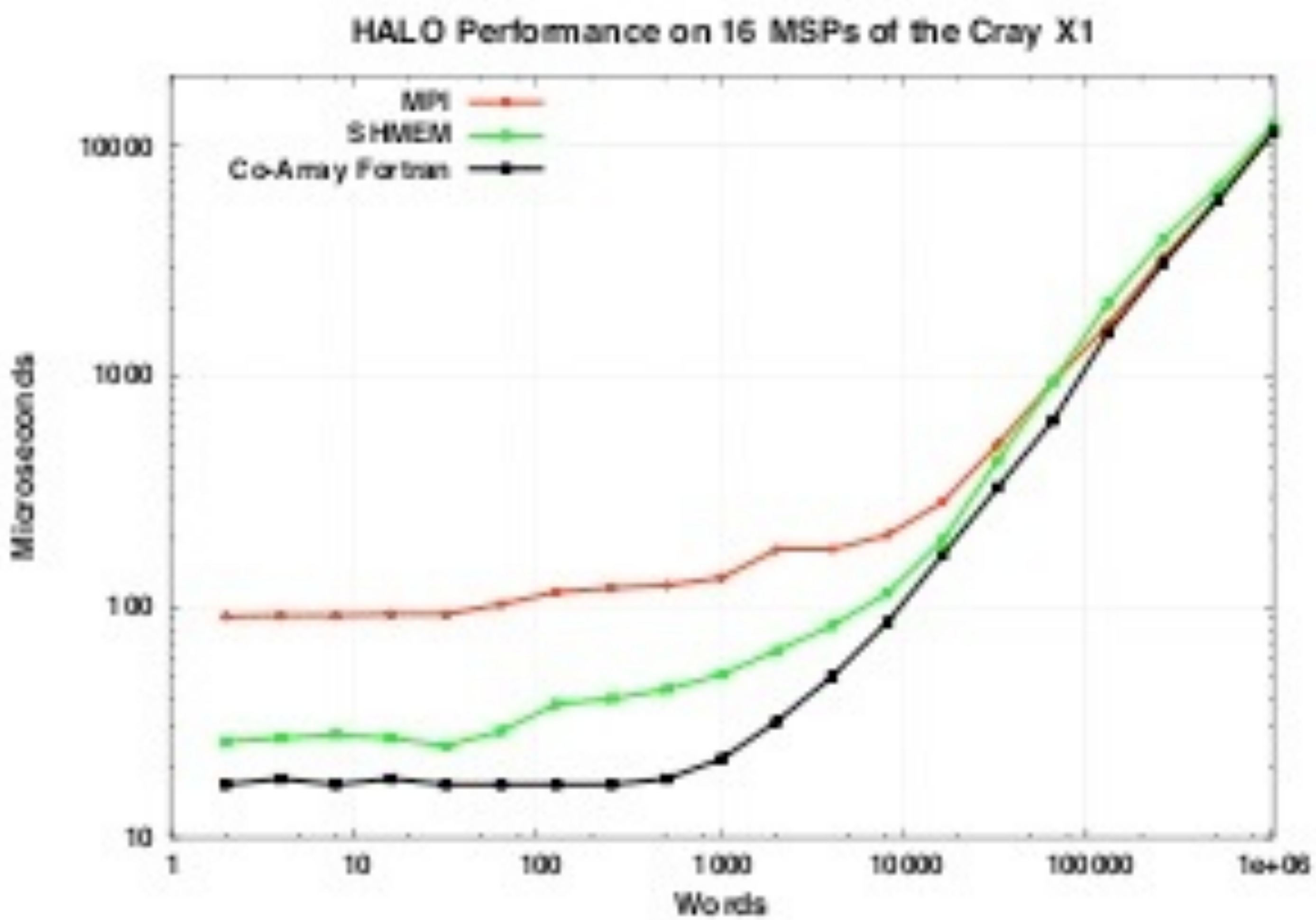
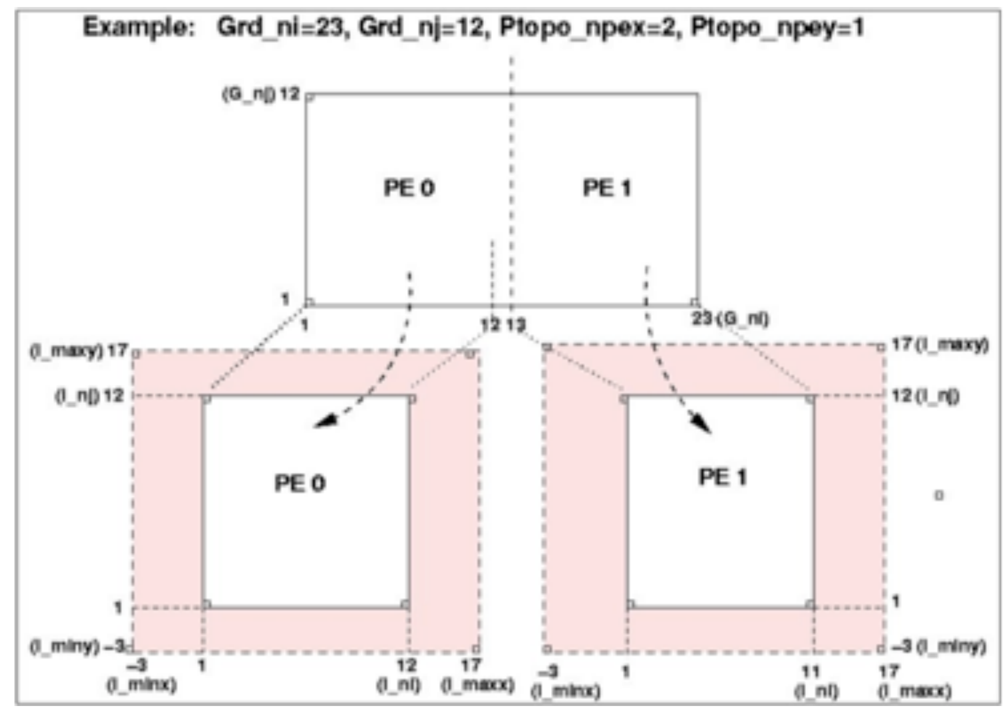


Halo Exchange “Stencil 2D” Benchmark



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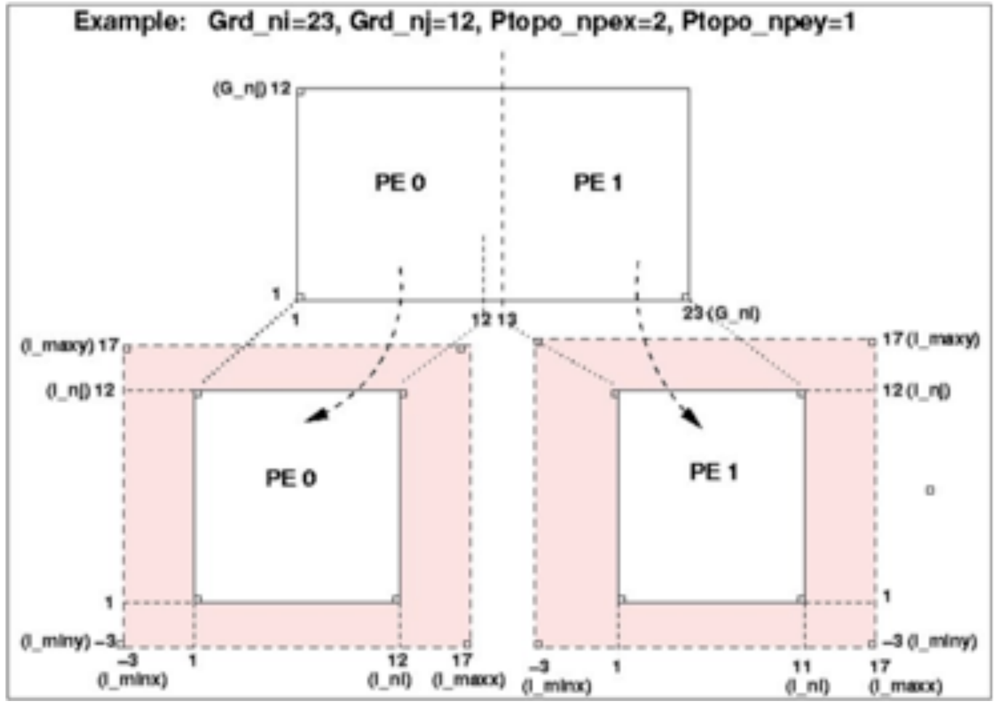
Halo exchange and stencil operation over a square domain distributed over a 2-D virtual process topology



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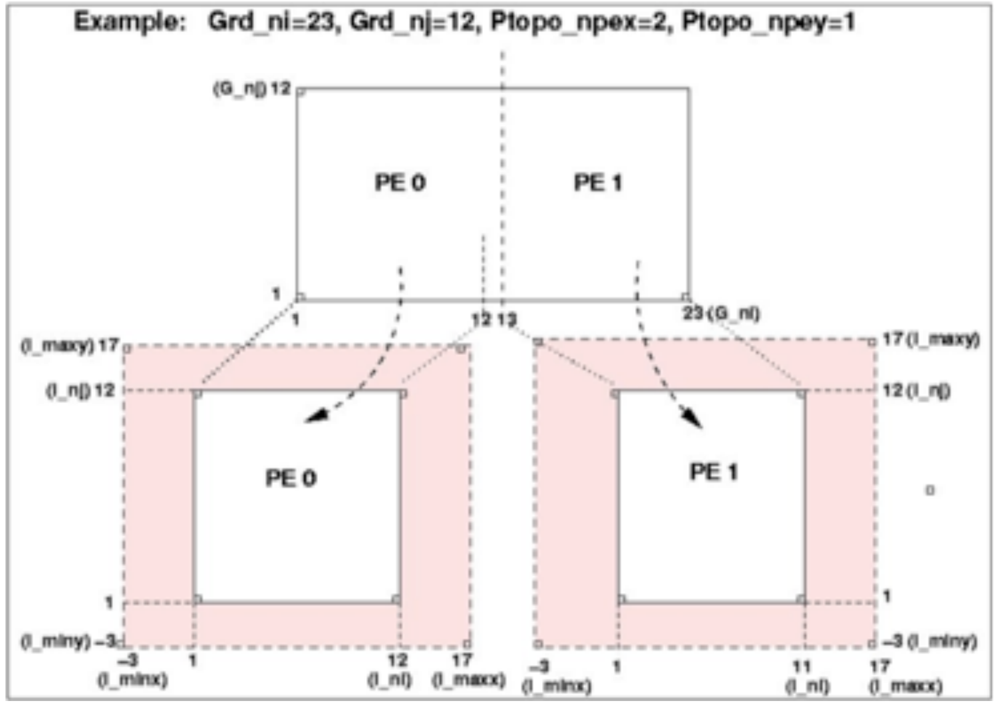
- Arbitrary halo ‘radius’ (number of halo cells in a given dimension, e.g. 3)



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- Arbitrary halo ‘radius’ (number of halo cells in a given dimension, e.g. 3)
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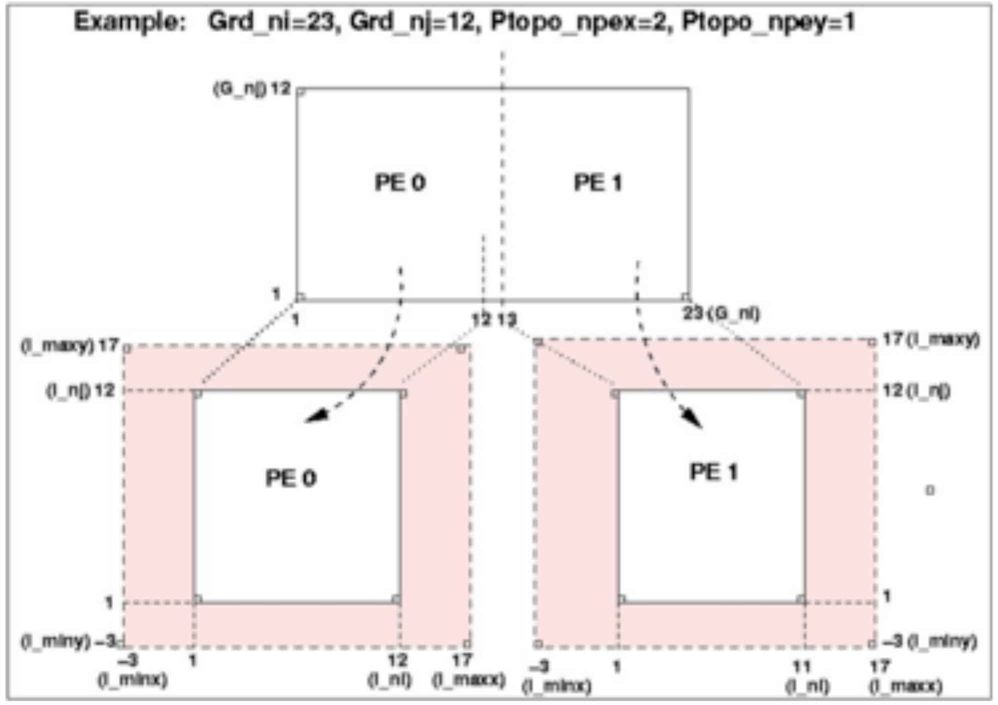
  - Trivial: post all 8 MPI_Isend and Irecv
  - Sendrecv: MPI_Sendrecv between PE pairs
  - Halo: MPI_Isend/Irecv between PE pairs



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- MPI implementations:
  - Trivial: post all 8 MPI_Isend and Irecv
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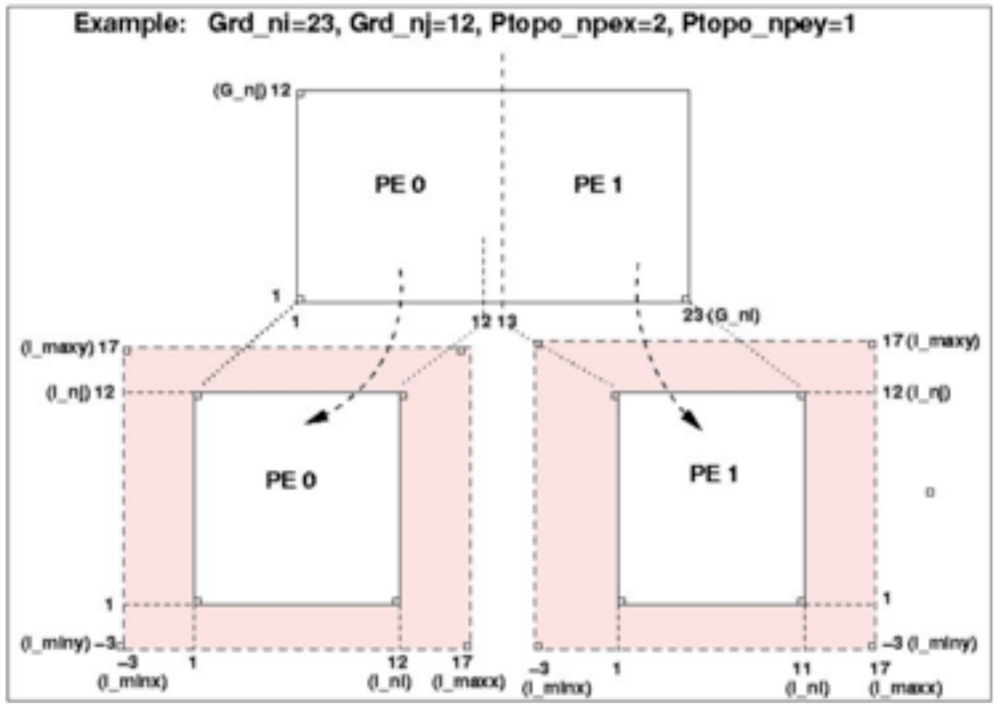
- CAF implementations:
  - Trivial: simple copies to remote images
  - Put: reciprocal puts between image pairs
  - Get: reciprocal gets between image pairs
  - Get0: all images do inner region first, then all do block region (fine grain, no sync.)
  - Get1: half of images do inner region first,half do block region first (fine grain, no sync.)



Example code: Trivial CAF

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```
     real, allocatable, save :: V(:,:)[:,:]
  :
 allocate( V(1-halo:m+halo,1-halo:n+halo)[p,*] )
  :
 WW = myP-1 ; if (WW<1) WW = p
 EE = myP+1 ; if (EE>p) EE = 1
 SS = myQ-1 ; if (SS<1) SS = q
 NN = myQ+1 ; if (NN>q) NN = 1
   :

 V(1:m,1:n)                        = dom(1:m,1:n)               !  computational region

 V(1-halo:0, 1:n)[EE,myQ]          = dom(m-halo+1:m,1:n)        !  to East
 V(m+1:m+halo, 1:n)[WW,myQ]        = dom(1:halo,1:n)            !  to West
 V(1:m,1-halo:0)[myP,NN]           = dom(1:m,n-halo+1:n)        !  to North
 V(1:m,n+1:n+halo)[myP,SS]         = dom(1:m,1:halo)            !  to South
 V(1-halo:0,1-halo:0)[EE,NN]       = dom(m-halo+1:m,n-halo+1:n) !  to North-East
 V(m+1:m+halo,1-halo:0)[WW,NN]     = dom(1:halo,n-halo+1:n)     !  to North-West
 V(1-halo:0,n+1:n+halo)[EE,SS]     = dom(m-halo+1:m,1:halo)     !  to South-East
 V(m+1:m+halo,n+1:n+halo)[WW,SS]   = dom(1:halo,1:halo)         !  to South-West

 sync all
!
! Now run a stencil filter over the computational region (the region unaffected by halo values)
!
 do j=1,n
   do i=1,m
     sum = 0.
     do l=-halo,halo
       do k=-halo,halo
         sum = sum + stencil(k,l)*V(i+k,j+l)
       enddo
     enddo
     dom(i,j) = sum
   enddo
 enddo
```

Example code: CAF Put

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```
      :
  V(1:m,1:n)                       = dom(1:m,1:n)               !  internal region

  V(1-halo:0, 1:n)[EE,myQ]         = dom(m-halo+1:m,1:n)        !  to East
   :
  V(m+1:m+halo,n+1:n+halo)[WW,SS]  = dom(1:halo,1:halo)         !  to South-West

! NO GLOBAL SYNCHRONIZATION HERE
! Perform filter over exclusive region only
  do j=1+halo,n-halo
    do i=1+halo,m-halo
      sum = 0.
      do l=-halo,halo
        do k=-halo,halo
          sum = sum + stencil(k,l)*V(i+k,j+l)
        enddo
      enddo
      dom(i,j) = sum
    enddo
  enddo

! Pair-wise handshake synchronization
  do mode=0,1
    if ( mod(myP,2) == mode ) then
      sync images( (myQ-1)*p+WW )    ! West

      do j=1+halo,n-halo
        do i=1,halo
! Apply filter
            dom(i,j) = sum
        enddo
      enddo
    else
      sync images( (myQ-1)*p+EE )    ! East
      do j=1+halo,n-halo
        do i=m-halo+1,m
         :
```

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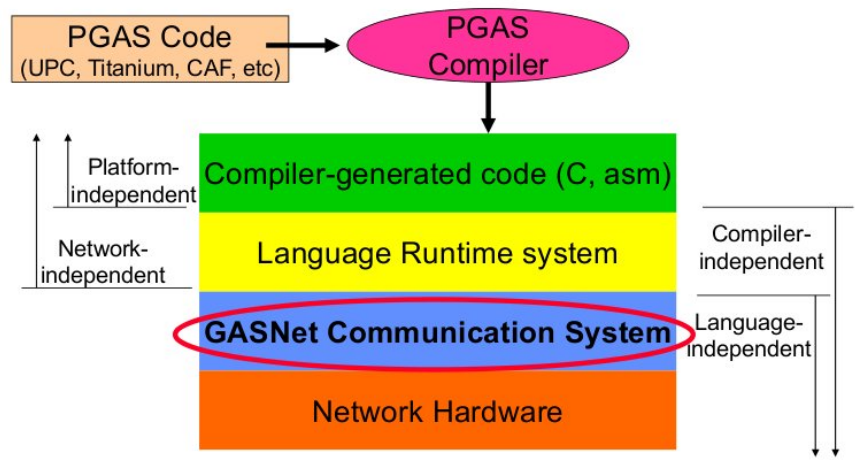

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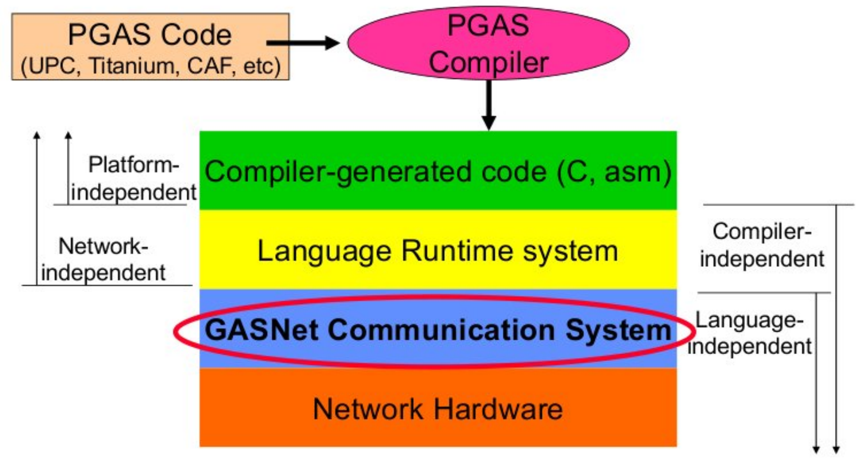

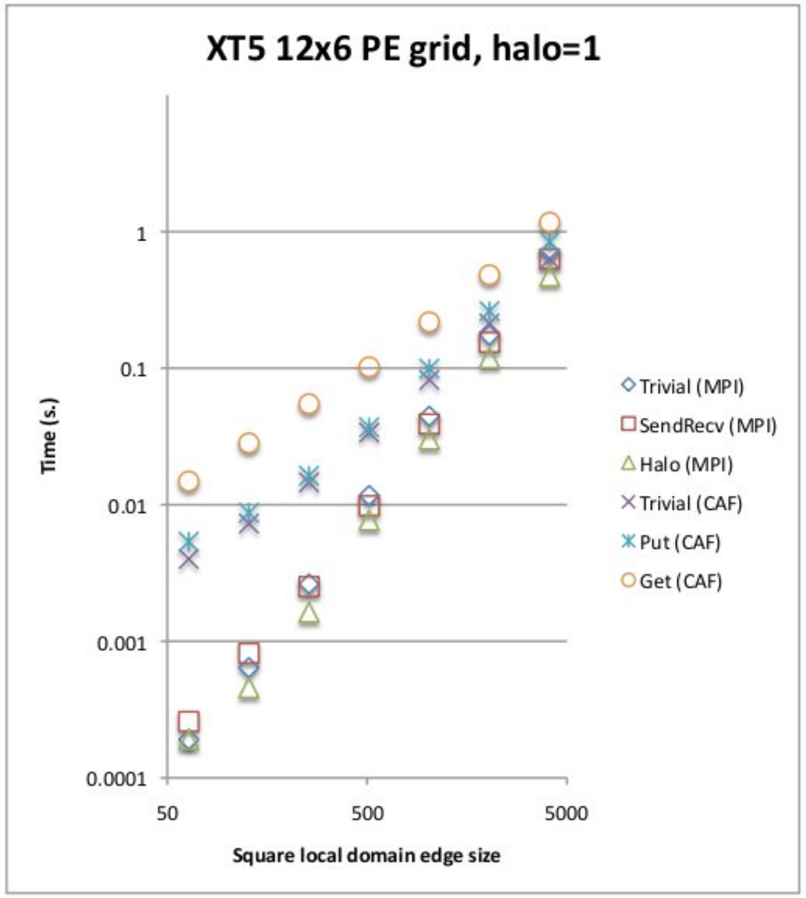

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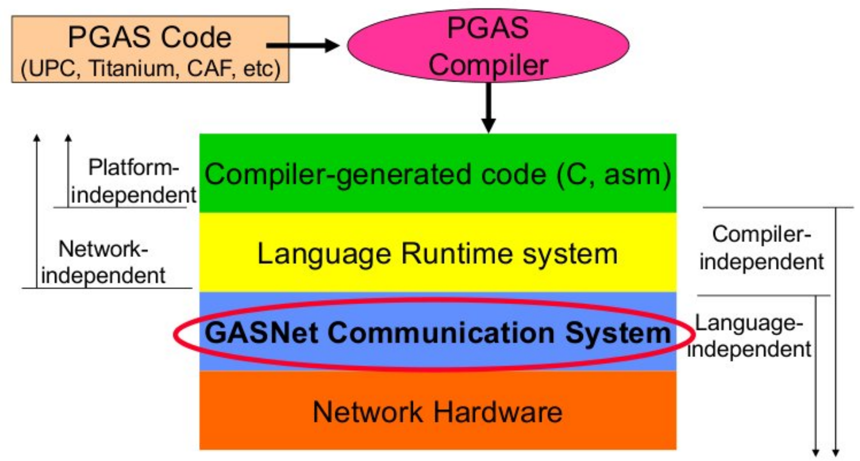

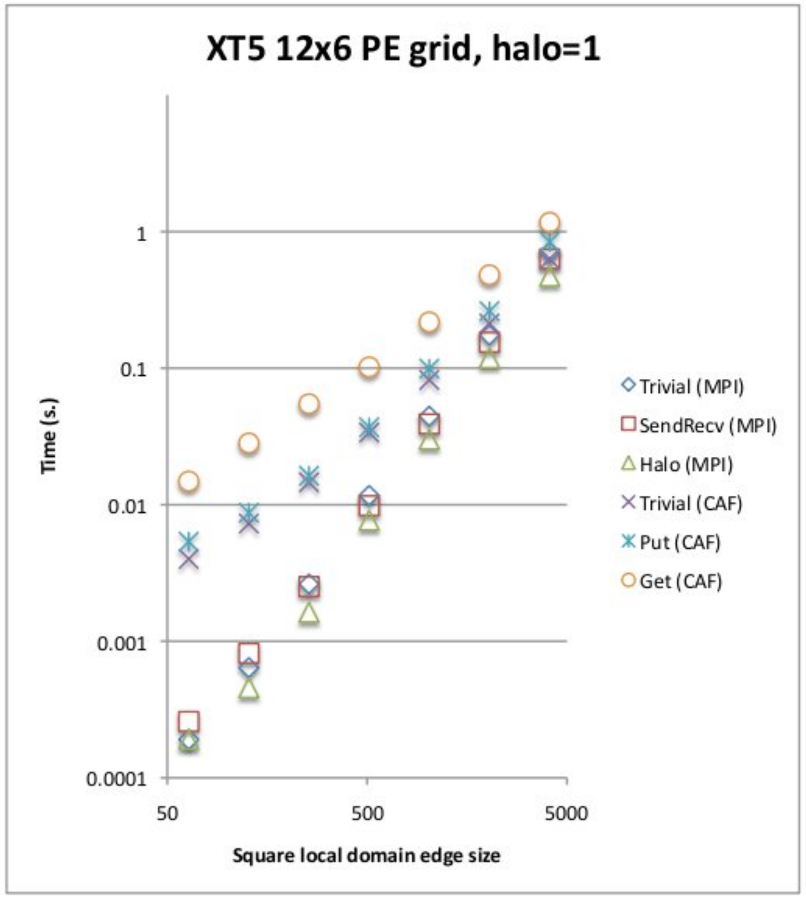

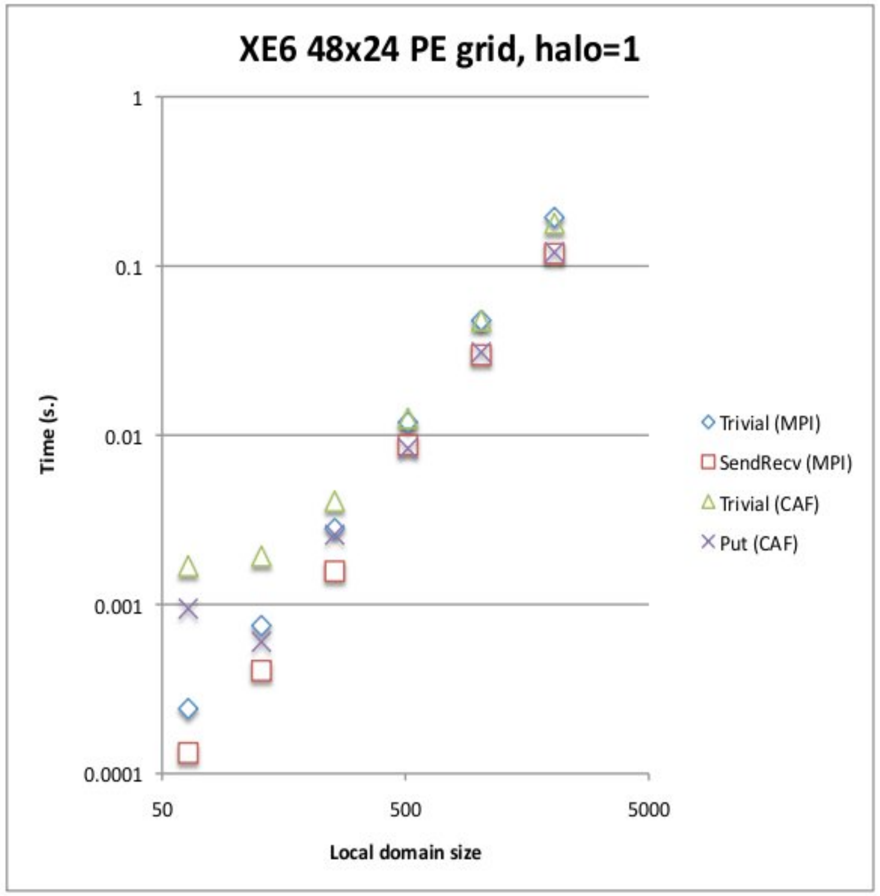

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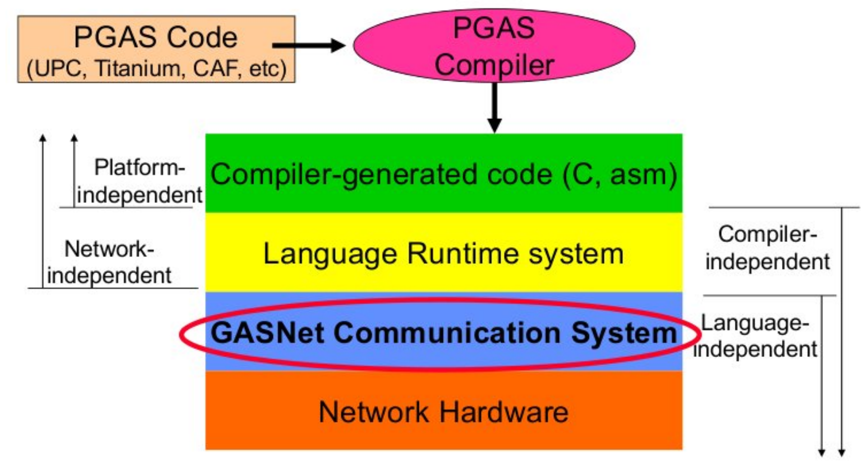

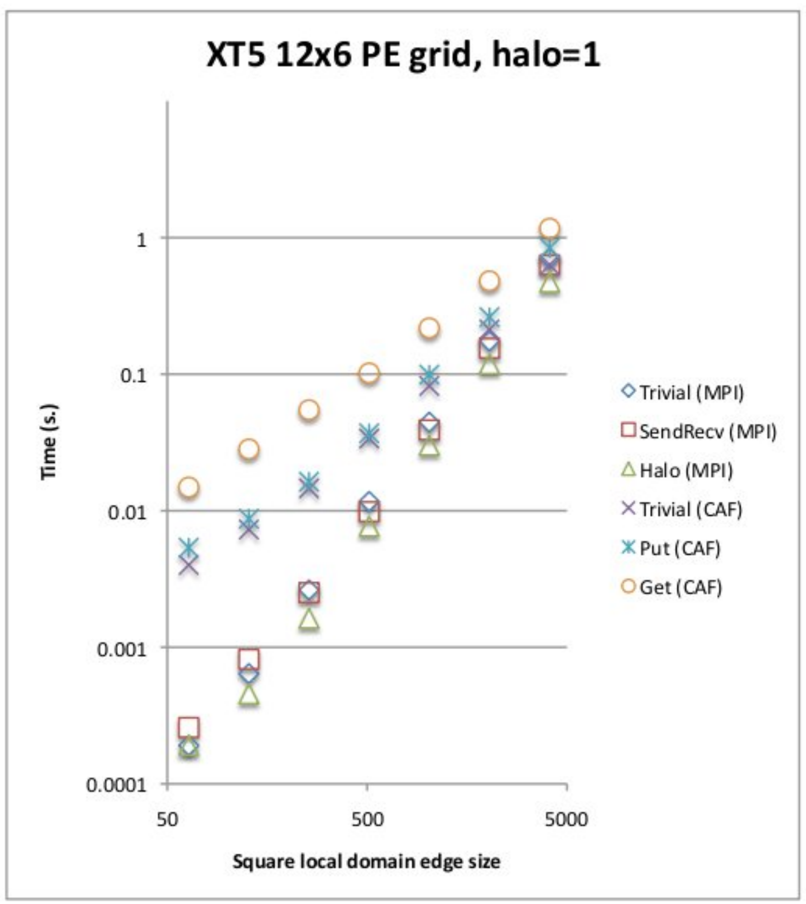

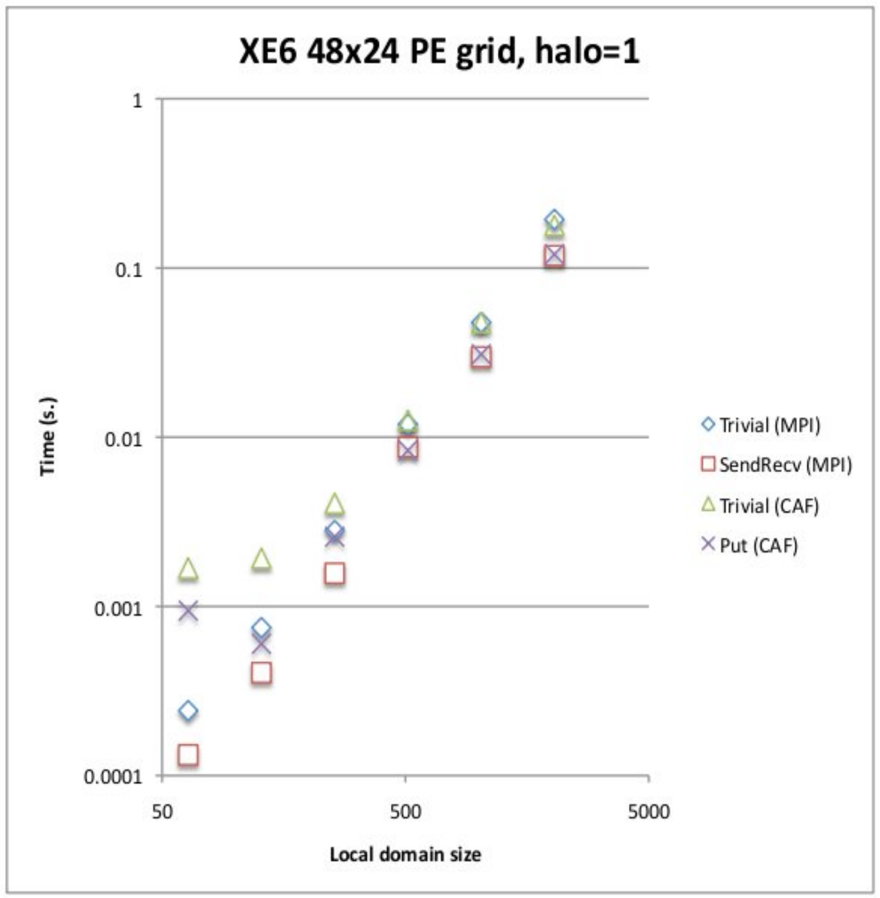

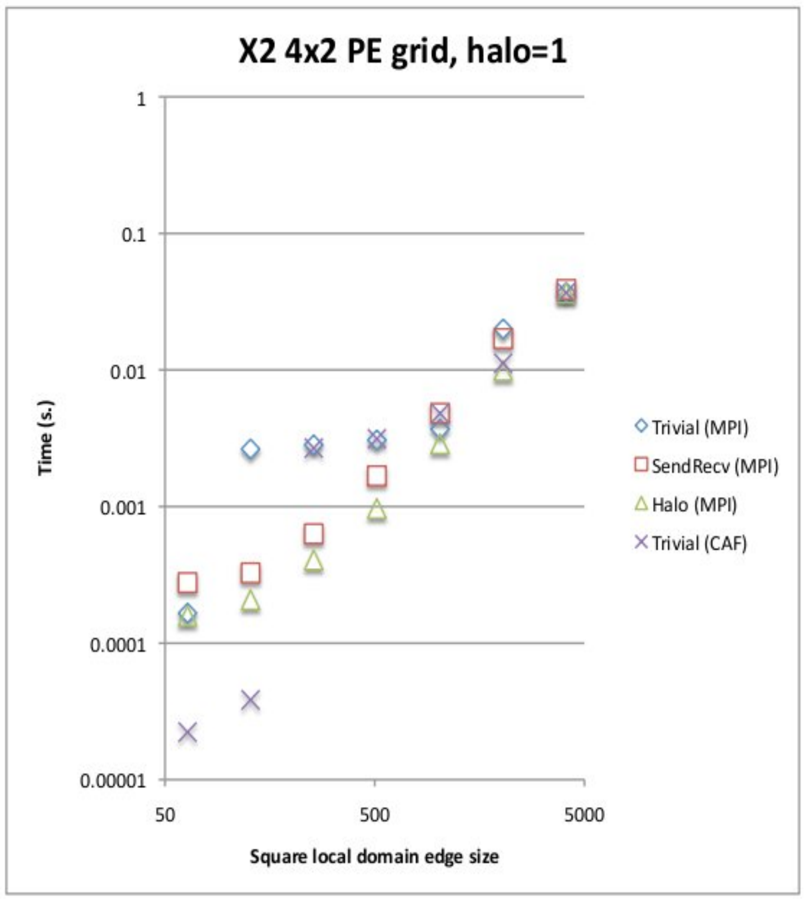

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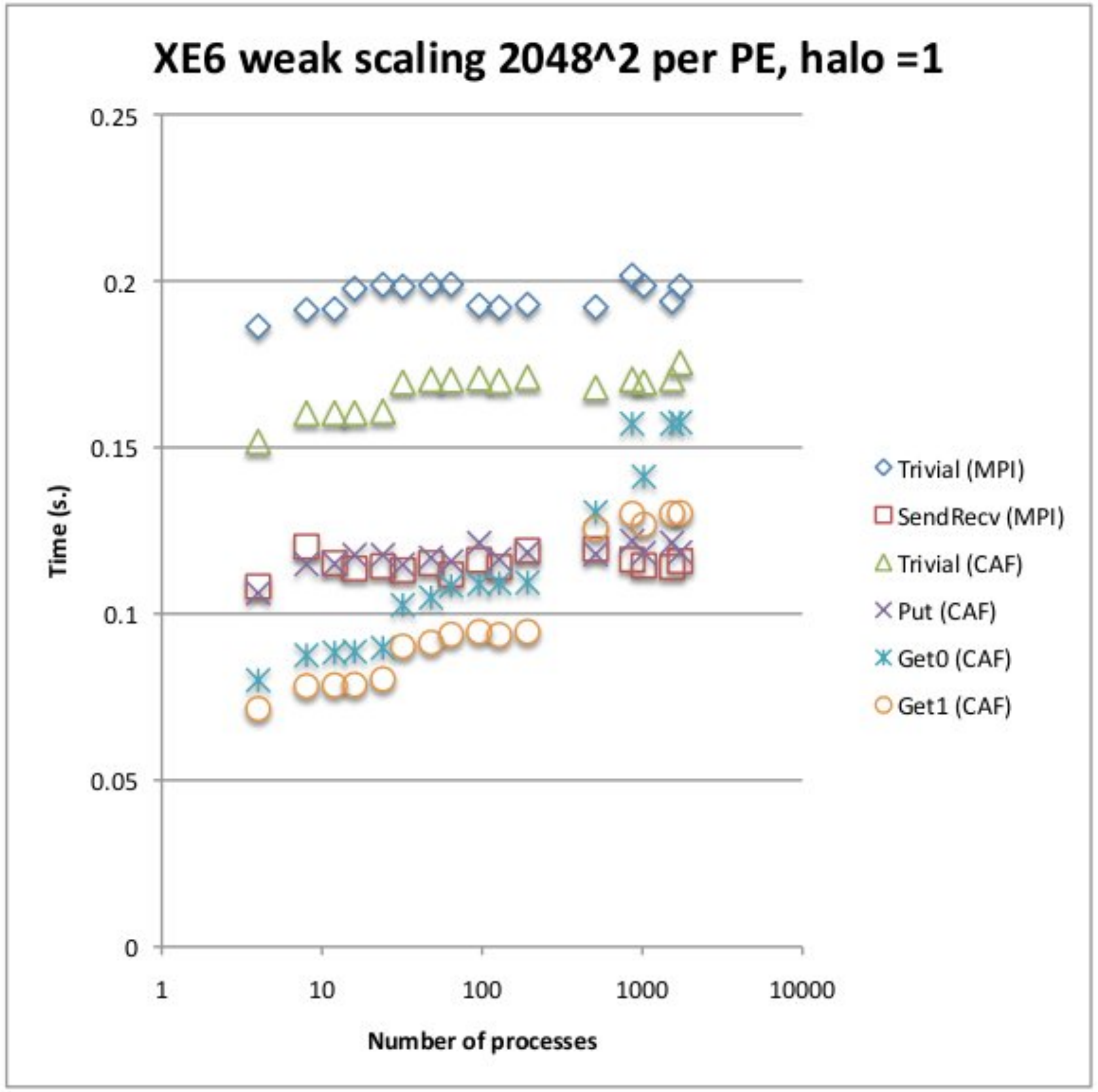

Friday, May 25, 2012

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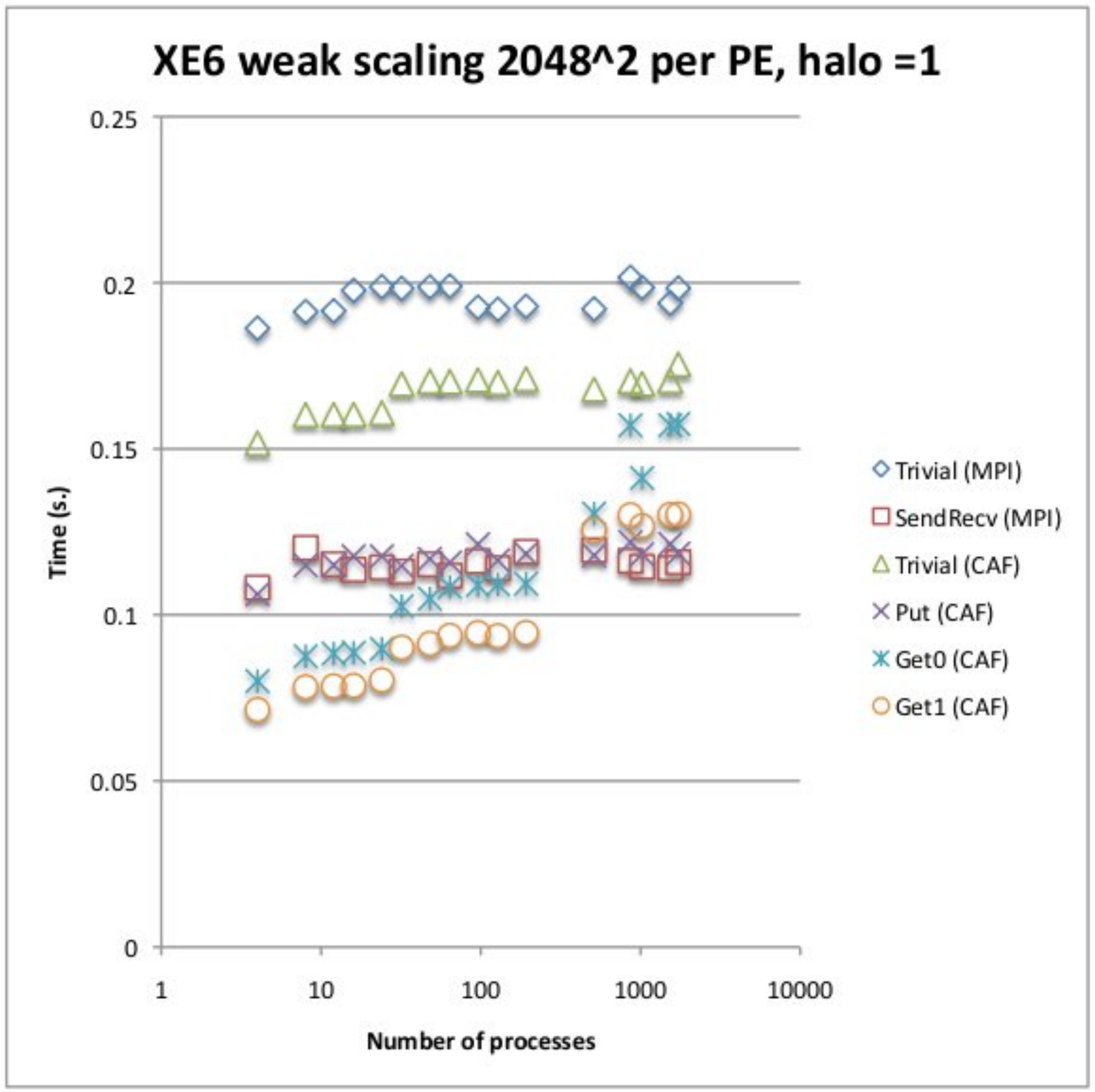

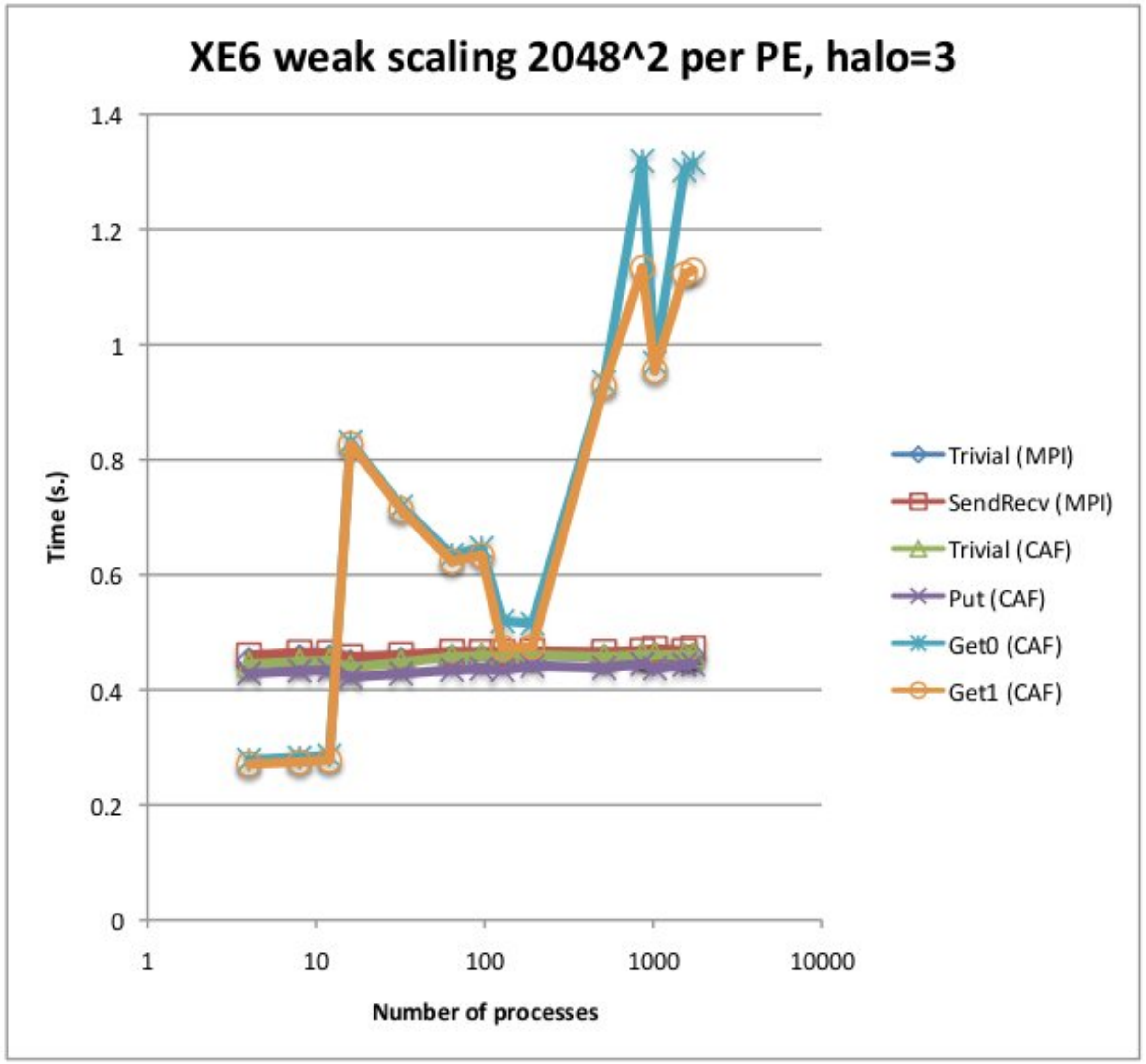

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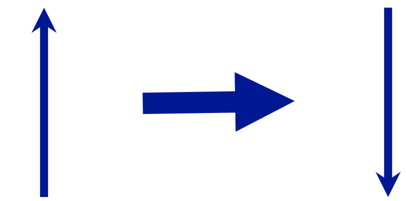

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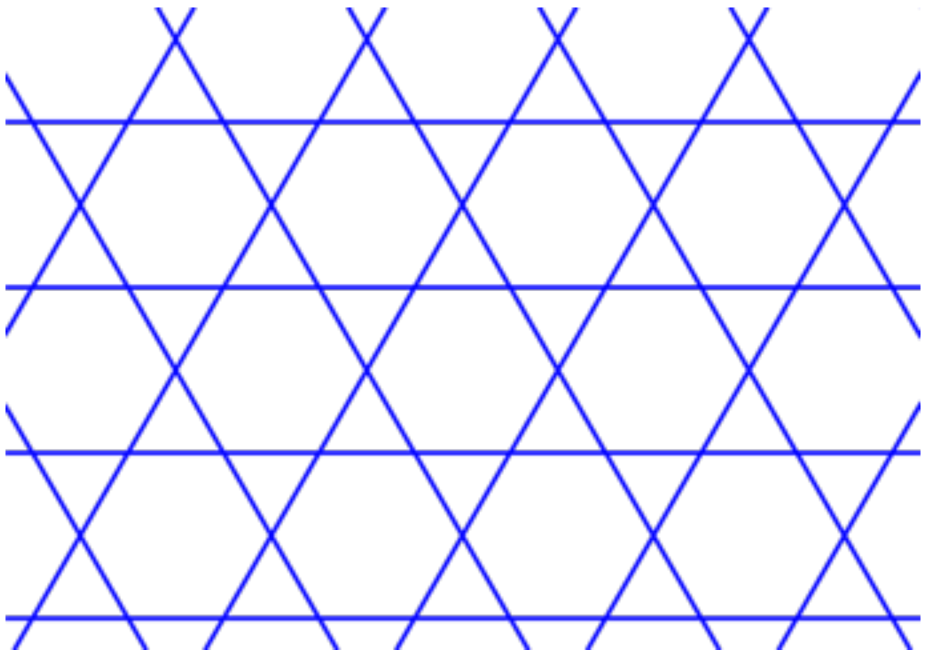

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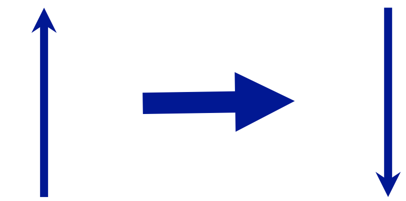

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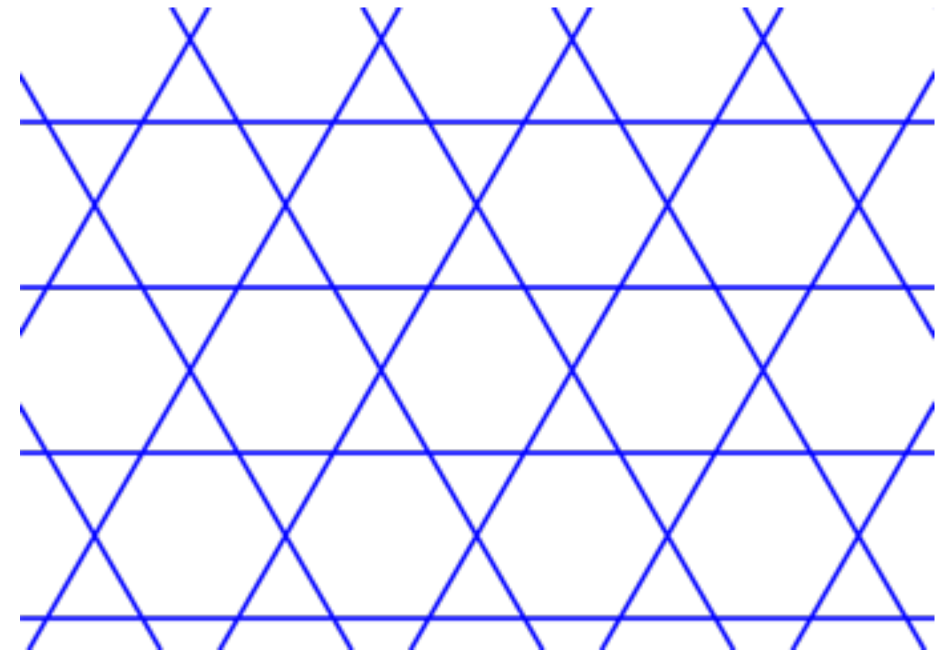

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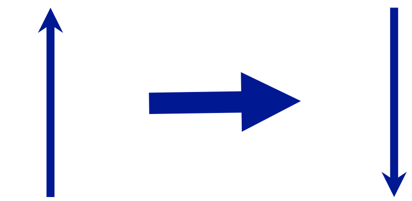
Problem 2: Exact Diagonalization



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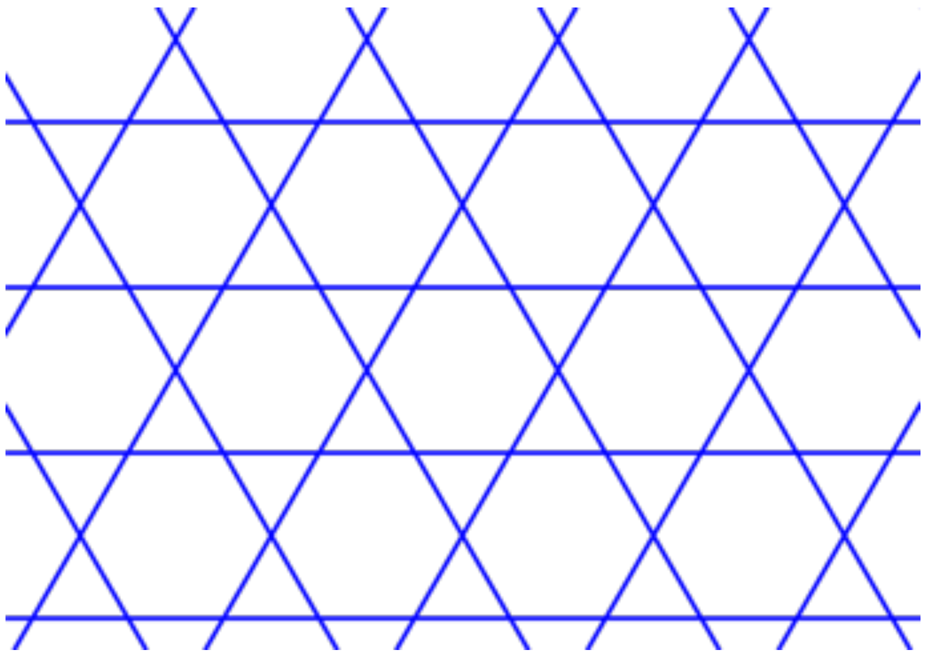

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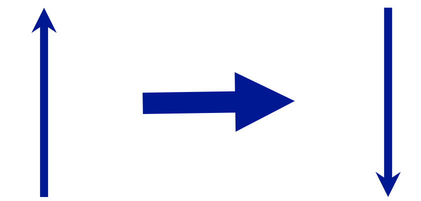

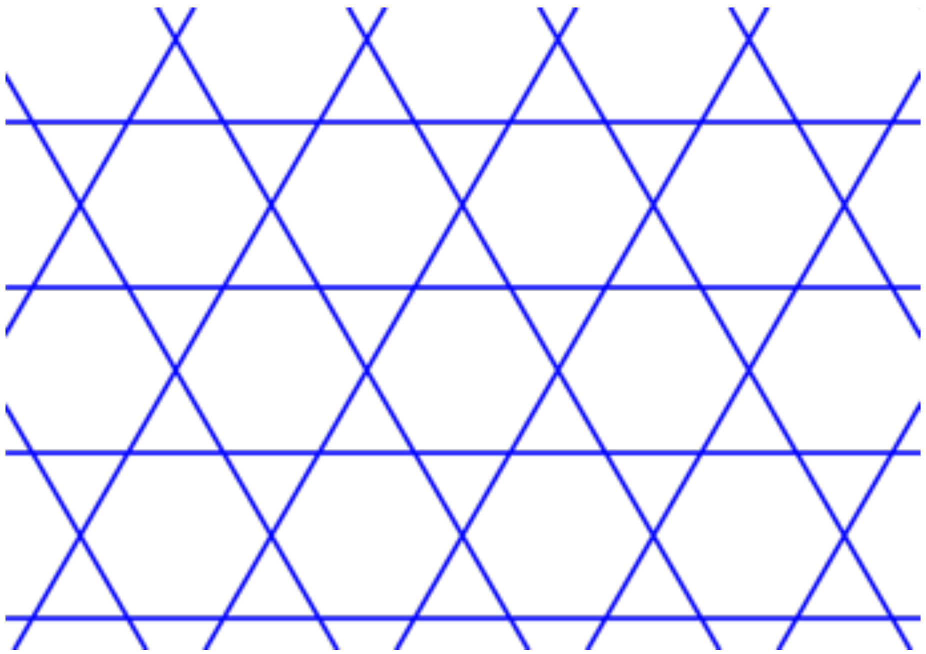

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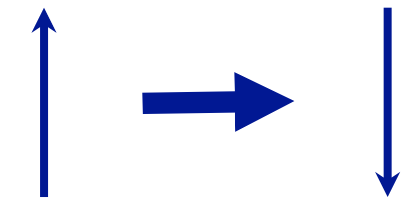

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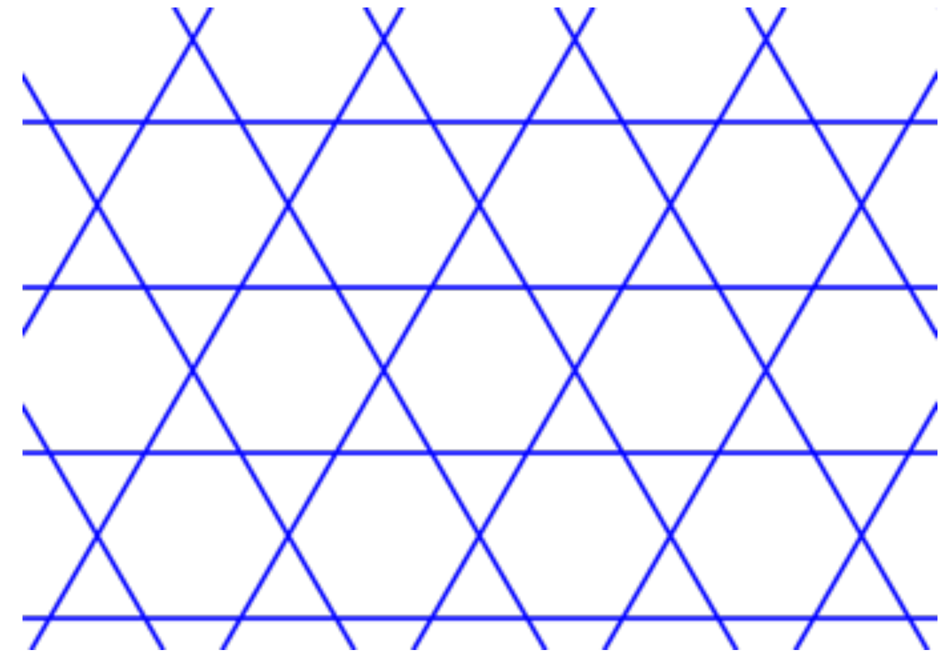

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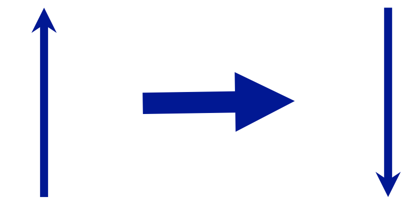

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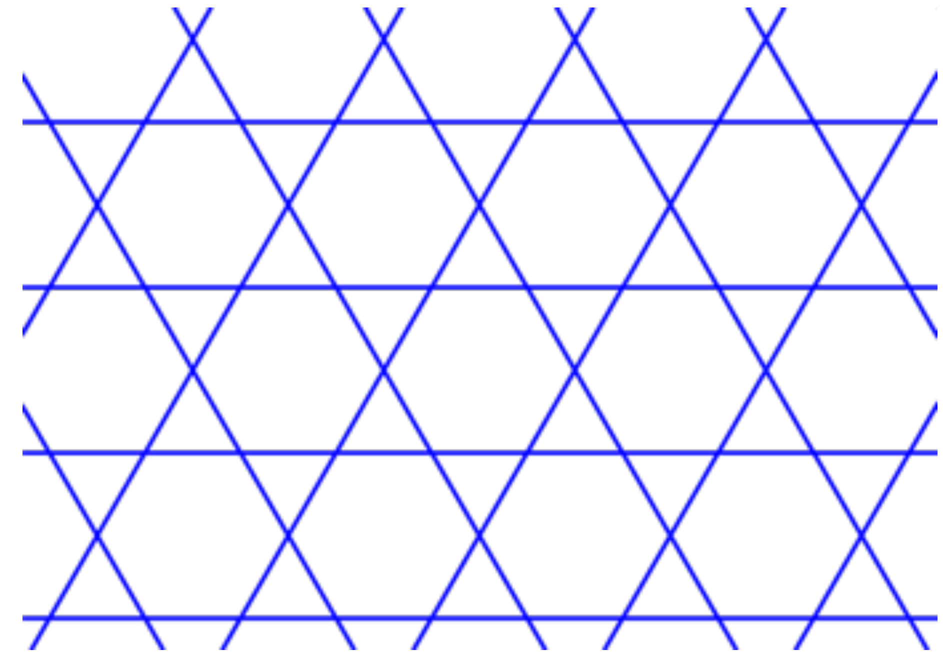

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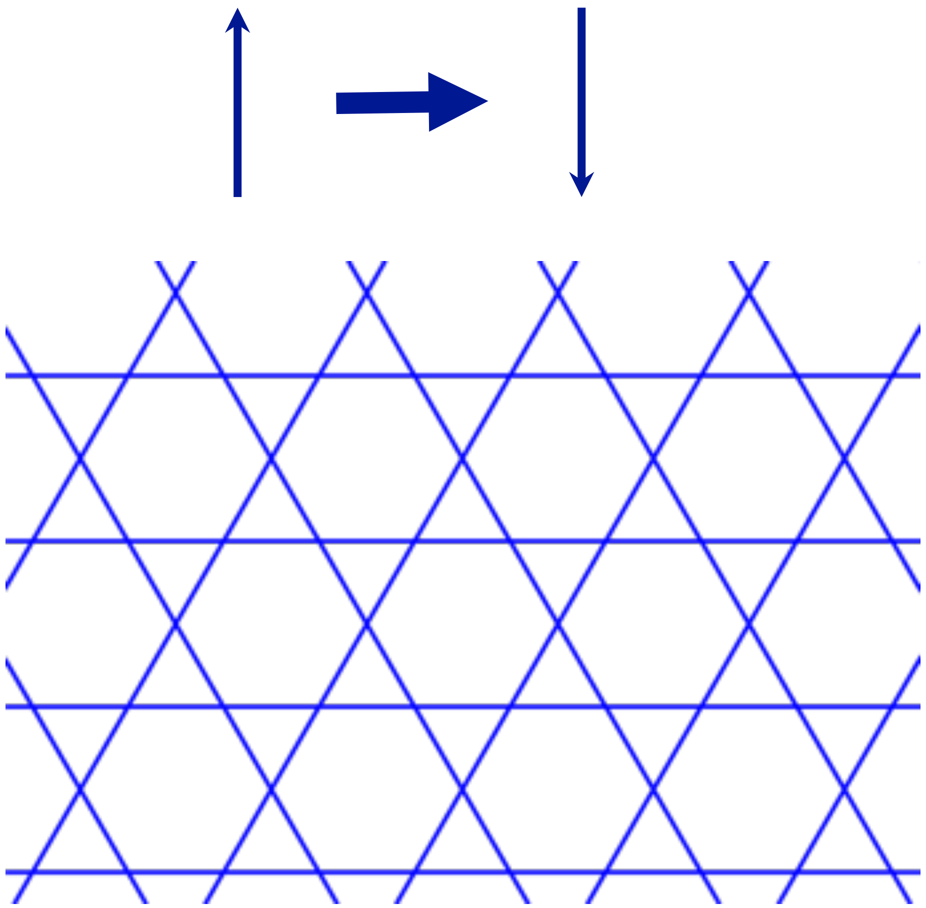
- Large, sparse symmetric mat-vec



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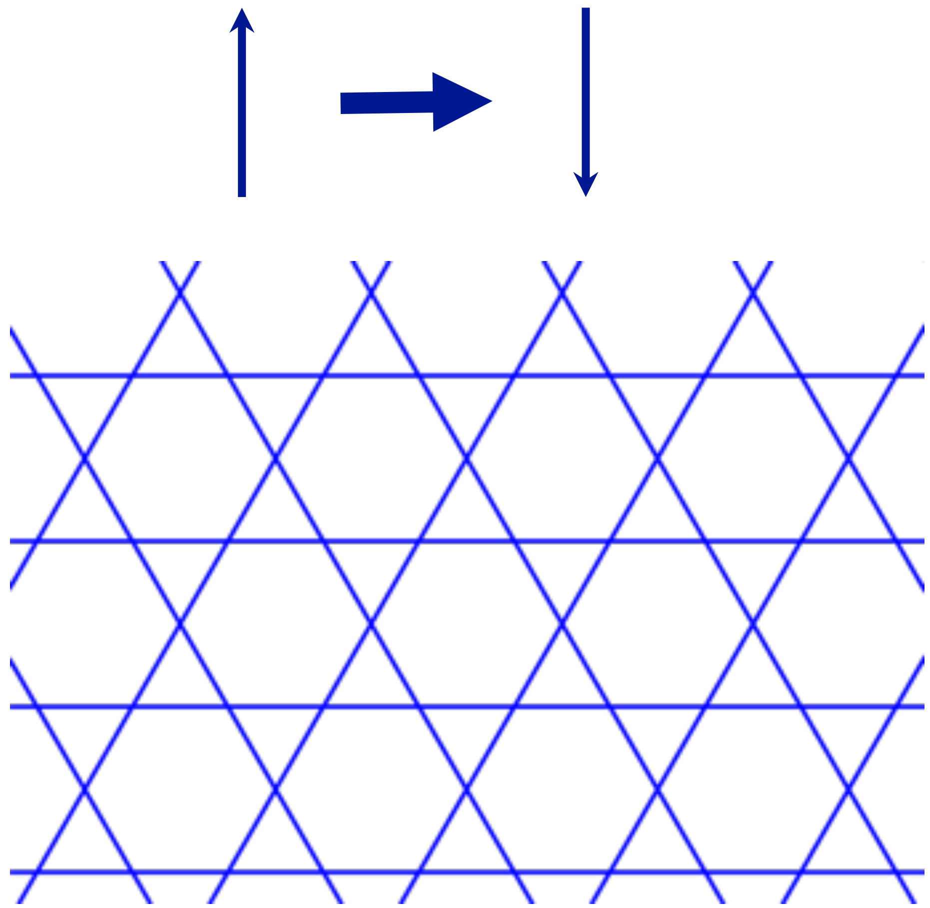

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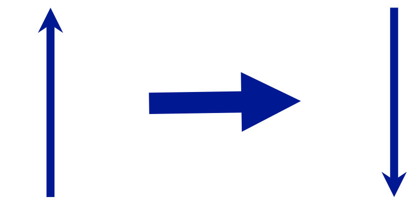

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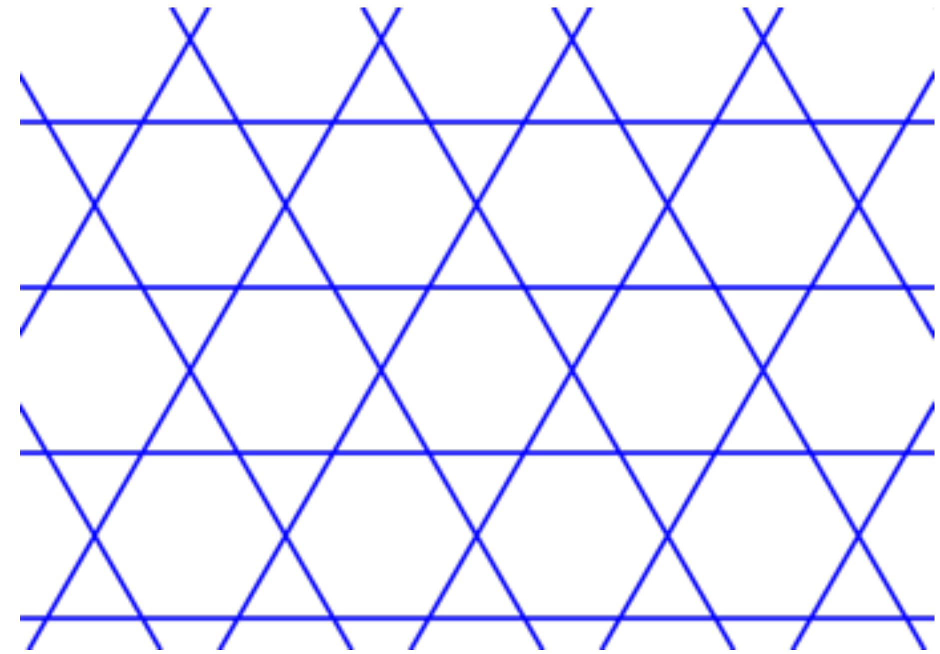

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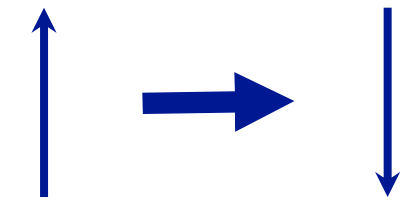

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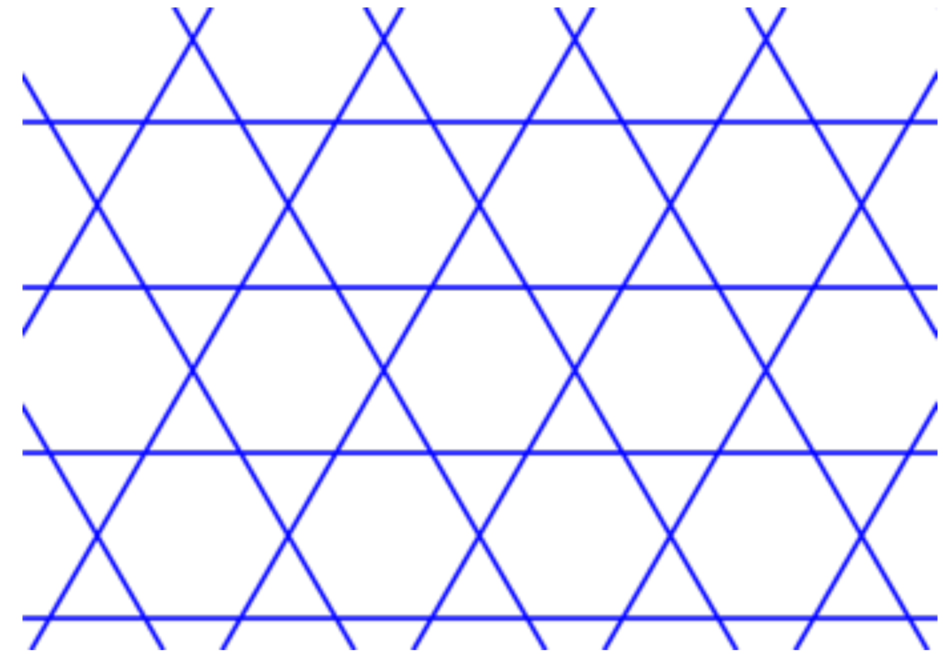

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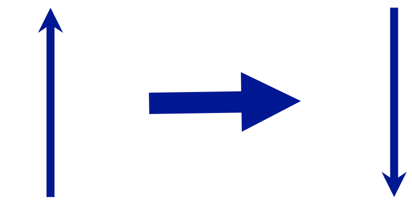

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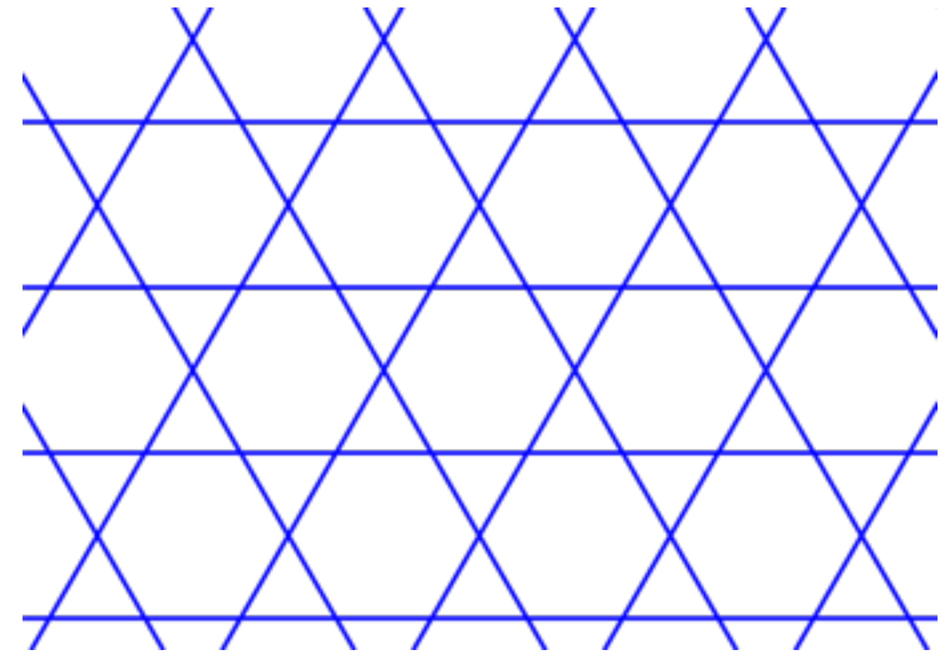

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Loop for MAX_ITER
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- **L3** (local work, normalize v1)
- **Loop over rounds of msgs**
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  - **L4** (work on local matrix, only 1st iteration)
  - **SYNC** (no-op, upc_fence)
  - **L7** (manage msg reception and do remote work)
- **L8** (local work, A norm)
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Code structure

```
void execute(ed){
  L1: for (i=0; i<2^(n-m); i++)
        b += v1[i]*v1[i]
  L2: for(iter=0; iter<max_iters; iter++)
        MPI_Barrier
        MPI_Allreduce of b
    L3: for (i=0; i<2^(n-m); i++)
          v1[i] *= f1(iter,b)
    MPI_Isend/MPI_Irecv to vv1 using handler1
    // local contribution, no comm
    L4: for (i=0; i<2^(n-m); i++)
          v2[i] = a(i)*v1[i]
          L5: for (k=0; k<n-m; k++)
                v2[i] += g*v1[f2(i,k)]
    // remote contribution, comm
    L6: for (k=n-m; k<n; k++) // m iterations
          MPI_Isend/MPI_Irecv to vv2 using handler2
          MPI_Wait on handler1
          L7: for (i=0; i<2^(n-m); i++)
                v2[i] += g*vv1[i]
          swap(vv1,vv2) // Pointer swap, no memcpy
          handler1 = handler2
    L8: for(i=0; i<2^(n-m); i++)
           a += v1[i]*v2[i]
        MPI_Barrier
        MPI_Allreduce of a
    L9: for(i=0; i<2^(n-m); i++)
          v2[i] = f3(i,iter,a)
          b += v2[i]*v2[i]
        swap (v0,v1,v2)
}
```

L3 L4 L6 L8 L9 execute

SPIN single core/socket/node comparisons

- Loop-based OMP directives: performance worse than MPI-only
- Task-based OpenMP/MPI implementation by Fourestey/Stringfellow

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System name	Rivera	Castor	Sandy
Processor	AMD 6274	Intel E5-2680	Intel X5650
Nickname	Interlagos	Westmere	Sandybridge
Cores/Socket	16	6	8
Sockets/Node	2	2	2
Hyperthreading	no	unenabled	yes (2)
Compiler	Open64	Intel	Intel
Core time (s.)	754 (1T)	280 (1T)	227 (1T)
Socket time (s.)	74 (15T)	51 (6T)	29 (16T)
Node time (s.)	38 (31T)	26 (12T)	15 (32T)

Multi-buffering concept

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Double buffering

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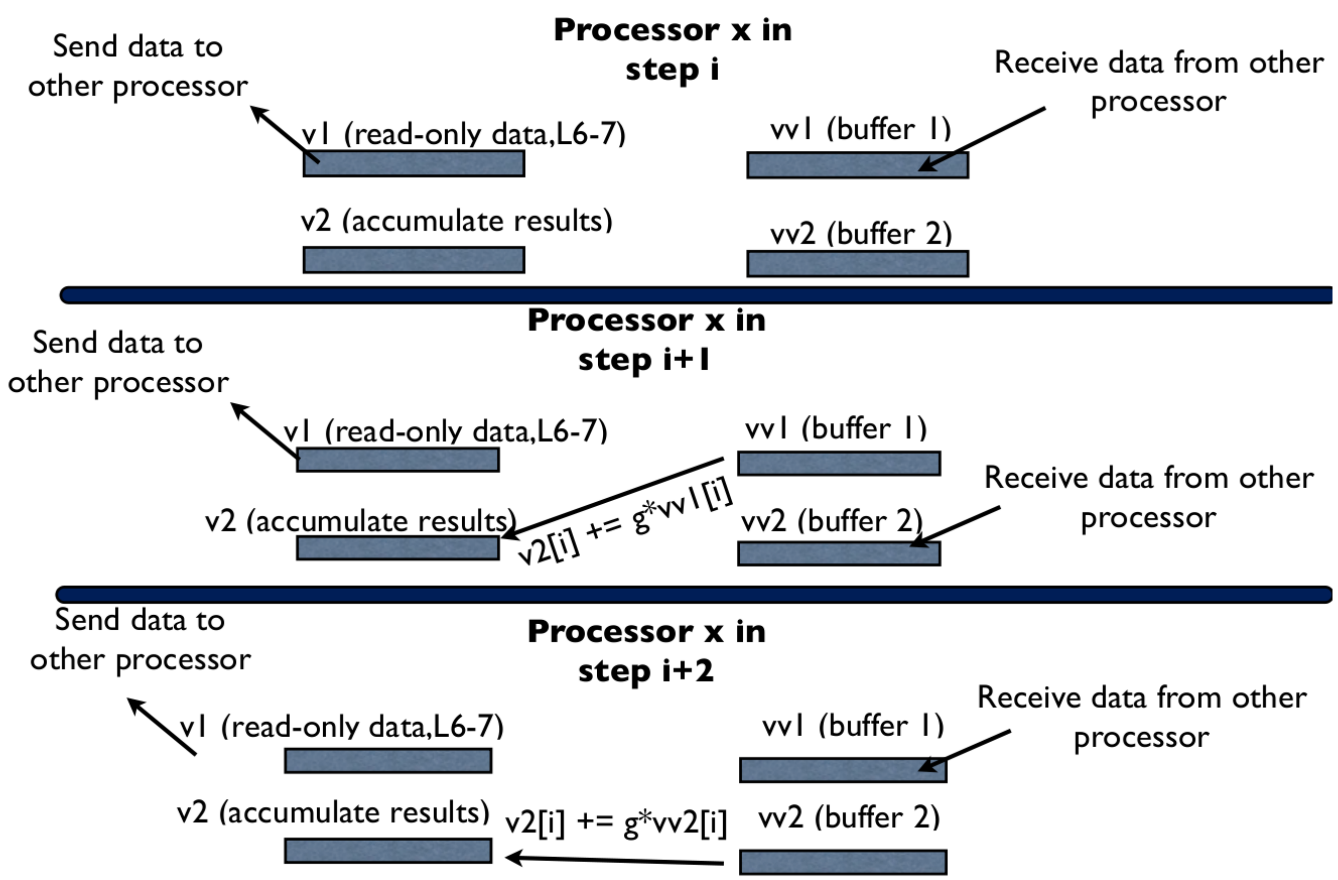
Double buffering



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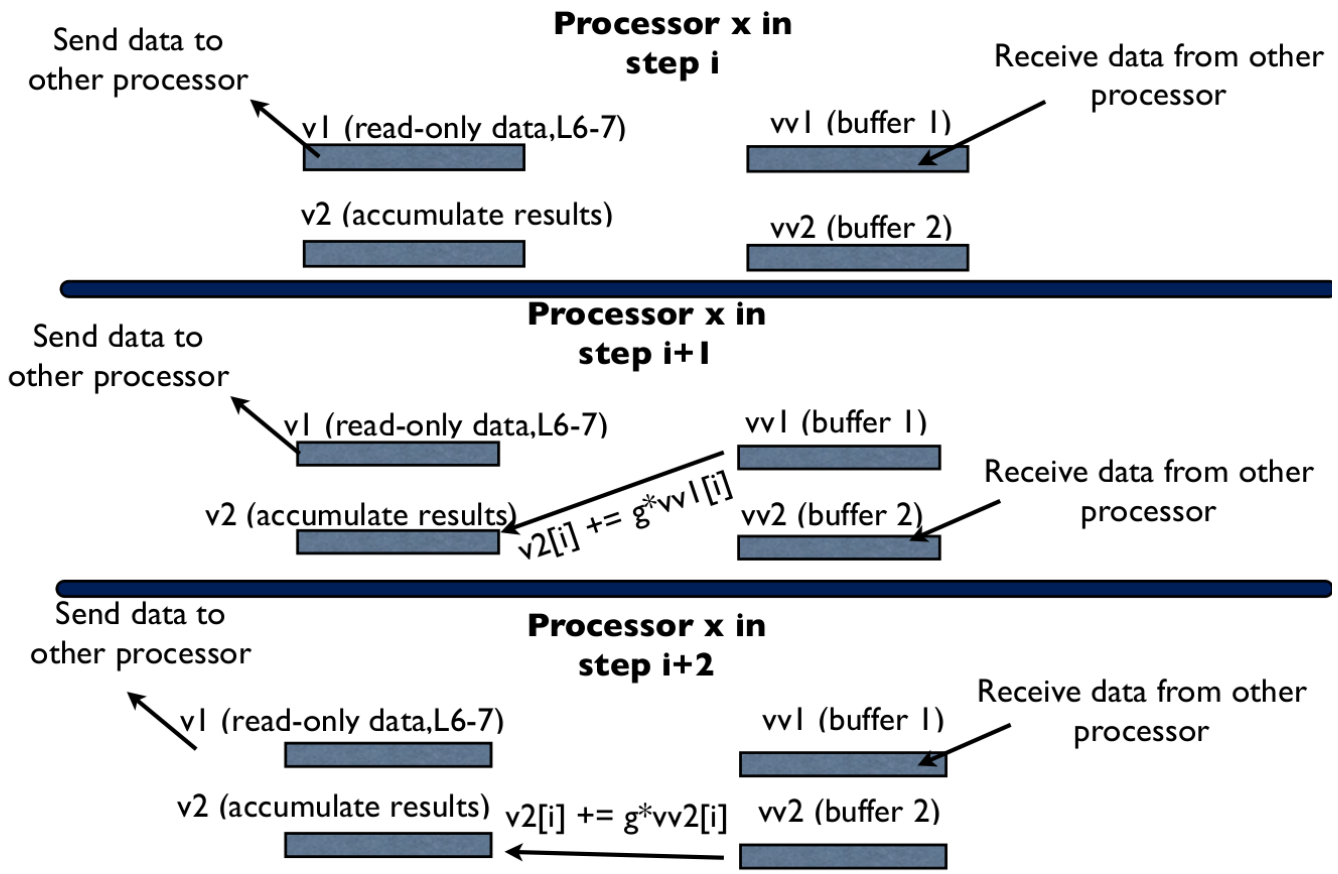

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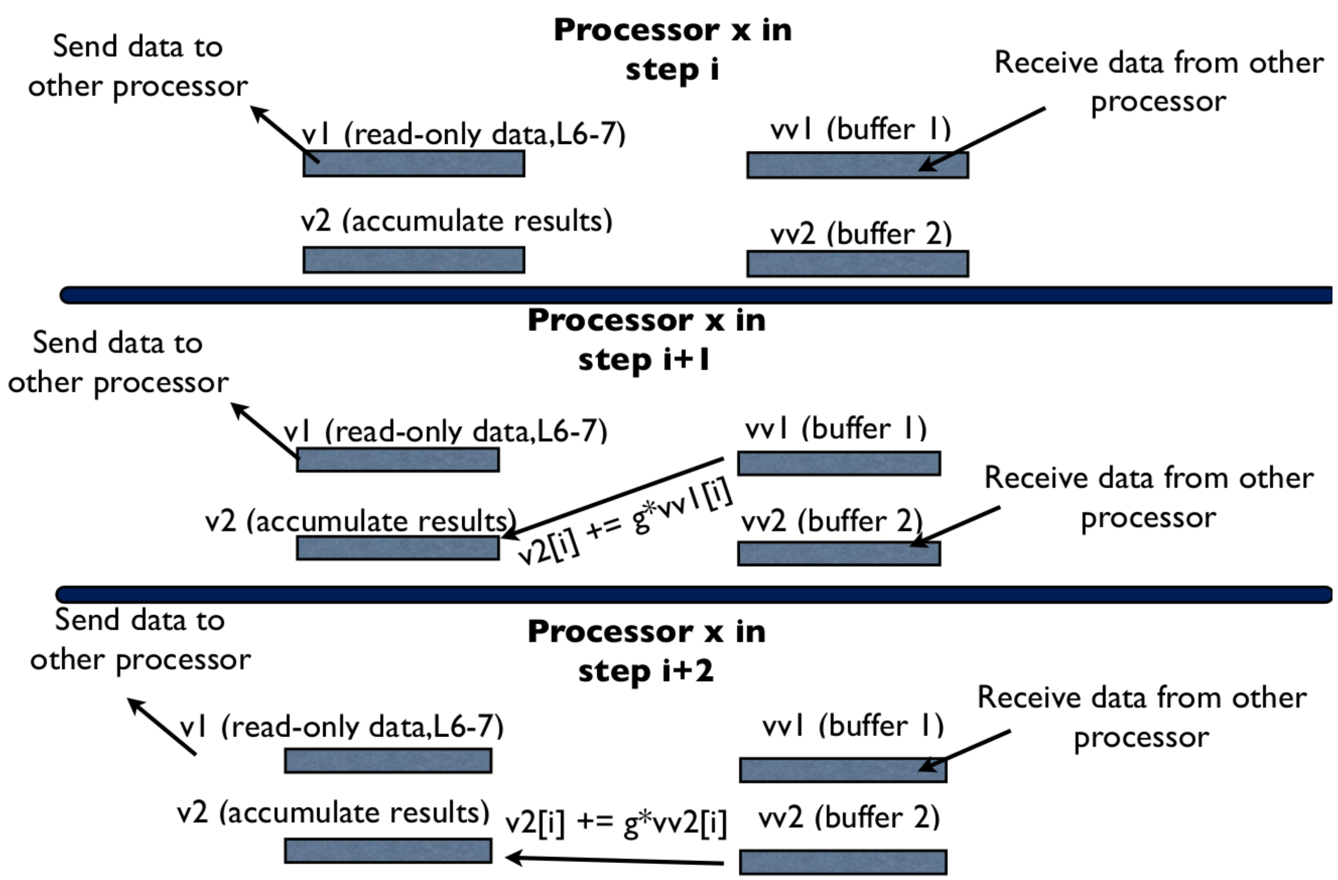

Multi-buffering

REFERENCE — 1 private buffer per pe

- Local work
- Loop
  - 2-sided MPI_Isend/Irecv (single round)
  - MPI_Wait
  - Remote work (in order)

OPTIMIZED — k shared buffers per pe (limited by on-node mem)

- Loop
  - 1-sided non-blocking put (round of k msgs)
  - Local work (if any)
  - Sync (e.g. barrier, fence, or notification flags)
  - Remote work (out of order)

Sequential Implementation

Sequential Implementation

```
struct ed_s { ...
        double *v0, *v1, *v2;       /* vectors */
        double *swap;               /* for swapping vectors */
};
              :
for (iter = 0; iter < ed->max_iter; ++iter) {
                 :
                /* matrix vector multiplication */
                for (s = 0; s < ed->nlstates; ++s ) {
                        /* diagonal part */
                        ed->v2[s] = diag(s, ed->n, ed->j) * ed->v1[s];
                        /* offdiagonal part */
                        for (k = 0; k < ed->n; ++k) {
                                s1 = flip_state(s, k);
                                ed->v2[s] += ed->gamma * ed->v1[s1];
                        }
                }
                 :
                /* Calculate alpha */
                /* Calculate beta */
        }
}
```

UPC “Elegant” Implementation

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```
struct ed_s { ...
        shared double *v0, *v1, *v2;        /* vectors */
        shared double *swap;                /* for swapping vectors */
};
              :
for (iter = 0; iter < ed->max_iter; ++iter) {
                :
                upc_barrier(0);
                /* matrix vector multiplication */
                upc_forall (s = 0; s < ed->nlstates; ++s; &(ed->v1[s]) ) {
                        /* diagonal part */
                        ed->v2[s] = diag(s, ed->n, ed->j) * ed->v1[s];
                        /* offdiagonal part */
                        for (k = 0; k < ed->n; ++k) {
                                s1 = flip_state(s, k);
                                ed->v2[s] += ed->gamma * ed->v1[s1];
                        }
                }
                :
                /* Calculate alpha */
                /* Calculate beta */
        }
}
```

Inelegant UPC versions

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Inelegant 1

```
shared[NBLOCK] double vtmp[THREADS*NBLOCK];
  :
for (i = 0; i < NBLOCK; ++i) vtmp[i+MYTHREAD*NBLOCK] = ed->v1[i];
upc_barrier(1);
for (i = 0; i < NBLOCK; ++i) ed->vv1[i] = vtmp[i+(ed->from_nbs[0]*NBLOCK)];
  :
upc_barrier(2);
```

Inelegant 2

```
shared[NBLOCK] double vtmp[THREADS*NBLOCK];
  :
upc_memput( &vtmp[MYTHREAD*NBLOCK], ed->v1, NBLOCK*sizeof(double) );
upc_barrier(1);
upc_memget( ed->vv1, &vtmp[ed->from_nbs[0]*NBLOCK], NBLOCK*sizeof(double) );
  :
upc_barrier(2);
```

UPC *Inelegant3:* use double buffers and upc_put

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```
shared[NBLOCK] double vtmp1[THREADS*NBLOCK];
shared[NBLOCK] double vtmp2[THREADS*NBLOCK];
:
upc_memput( &vtmp1[ed->to_nbs[0]*NBLOCK], ed->v1, NBLOCK*sizeof(double) );
upc_barrier(1);
:
 if ( mode == 0 ) {
   upc_memput( &vtmp2[ed->to_nbs[neighb]*NBLOCK], ed->v1, NBLOCK*sizeof(double) );
 } else {
   upc_memput( &vtmp1[ed->to_nbs[neighb]*NBLOCK], ed->v1, NBLOCK*sizeof(double) );
 }
  :
 if ( mode == 0 ) {
   for (i = 0; i < ed->nlstates; ++i) { ed->v2[i] += ed->gamma * vtmp1[i+MYTHREAD*NBLOCK]; }
   mode = 1;
 } else {
   for (i = 0; i < ed->nlstates; ++i) { ed->v2[i] += ed->gamma * vtmp2[i+MYTHREAD*NBLOCK]; }
   mode = 0;
 }
 upc_barrier(2);
```

Other message passing paradigms

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MPI-2: One-sided PUT

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```
MPI_Put(ed->v1, ed->nlstates, MPI_DOUBLE, ed->to_nbs[0], 0, ed->nlstates, MPI_DOUBLE, win1);
MPI_Win_fence( 0, win1);
```

Other message passing paradigms

MPI-2: One-sided PUT

```
MPI_Put(ed->v1, ed->nlstates, MPI_DOUBLE, ed->to_nbs[0], 0, ed->nlstates, MPI_DOUBLE, win1);
MPI_Win_fence( 0, win1);
```

SHMEM: non-blocking PUT

Other message passing paradigms

MPI-2: One-sided PUT

```
MPI_Put(ed->v1, ed->nlstates, MPI_DOUBLE, ed->to_nbs[0], 0, ed->nlstates, MPI_DOUBLE, win1);
MPI_Win_fence( 0, win1);
```

SHMEM: non-blocking PUT

```
vtmp1 = (double *) shmalloc(ed->nlstates*sizeof(double));
  :
shmem_barrier_all();
shmem_double_put_nb(vtmp1, ed->v1, ed->nlstates, ed->from_nbs[neighb], NULL);
```

Other message passing paradigms

MPI-2: One-sided PUT

```
MPI_Put(ed->v1, ed->nlstates, MPI_DOUBLE, ed->to_nbs[0], 0, ed->nlstates, MPI_DOUBLE, win1);
MPI_Win_fence( 0, win1);
```

SHMEM: non-blocking PUT

```
vtmp1 = (double *) shmalloc(ed->nlstates*sizeof(double));
  :
shmem_barrier_all();
shmem_double_put_nb(vtmp1, ed->v1, ed->nlstates, ed->from_nbs[neighb], NULL);
```

SHMEM “fast”: non-blocking PUT, local wait only

Other message passing paradigms

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```
ed->v1[ed->nlstates] = ((double) ed->rank); /* sentinel */
for (l = 0; l < ed->m; ++l) {
  offset = l*(ed->nlstates+1); /* Offset into buffer */
  shmem_double_put_nb(&vtmp[offset],ed->v1, ed->nlstates+1,ed->to_nbs[l],NULL);
}
          :
tag = vtmp[offset+ed->nlstates];
while (tag != (double) ed->from_nbs[k-ed->nm]) { /* spin */
  tag = vtmp[offset+ed->nlstates];
}
for (i = offset, j=0; i < offset+ed->nlstates; ++i, ++j) {
   ed->v2[j] += ed->gamma * vtmp[i];
}
vtmp[l*(ed->nlstates+1)+ed->nlstates]=((double)-1); /*reset*/
```

SPIN strong scaling: Cray XE6, n=22,24; 10 iter.

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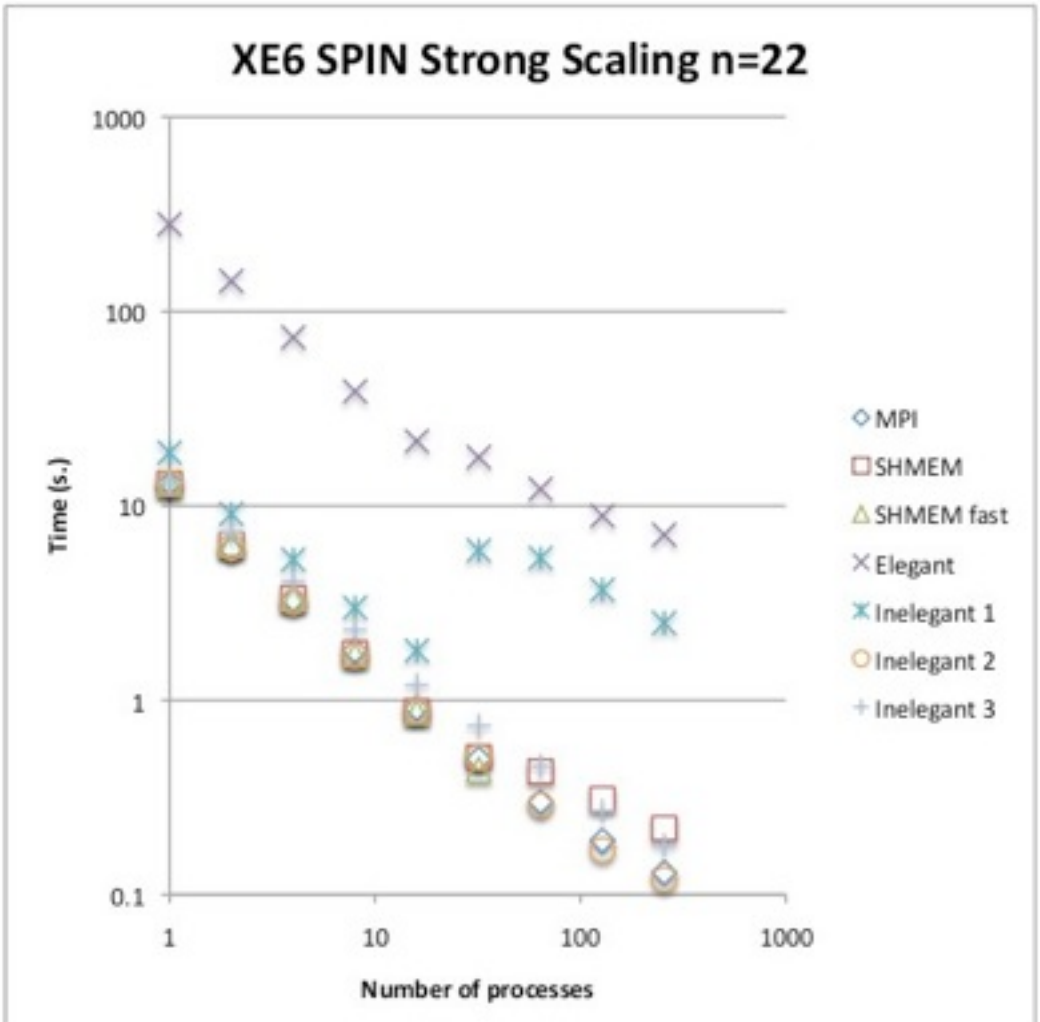

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSCS
Swiss National Supercomputing Centre

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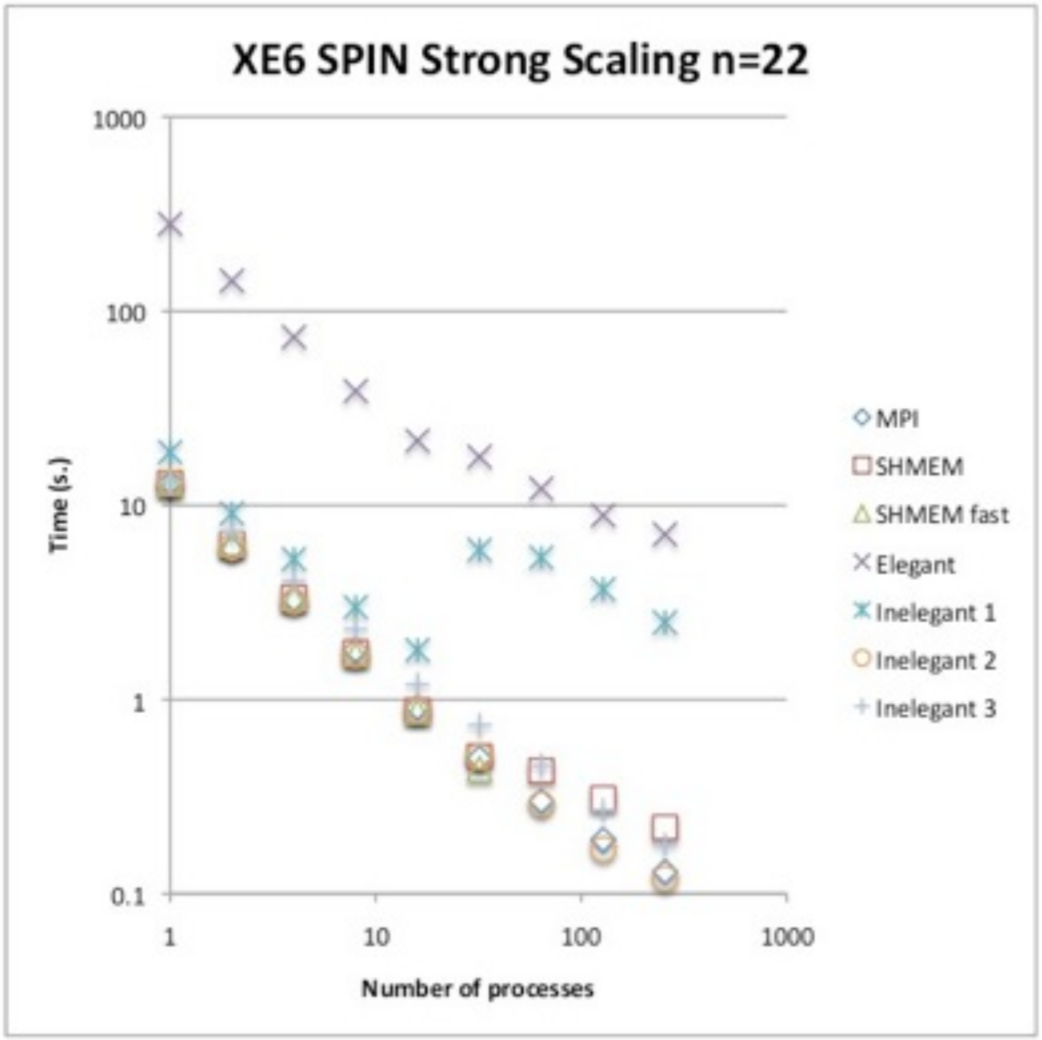

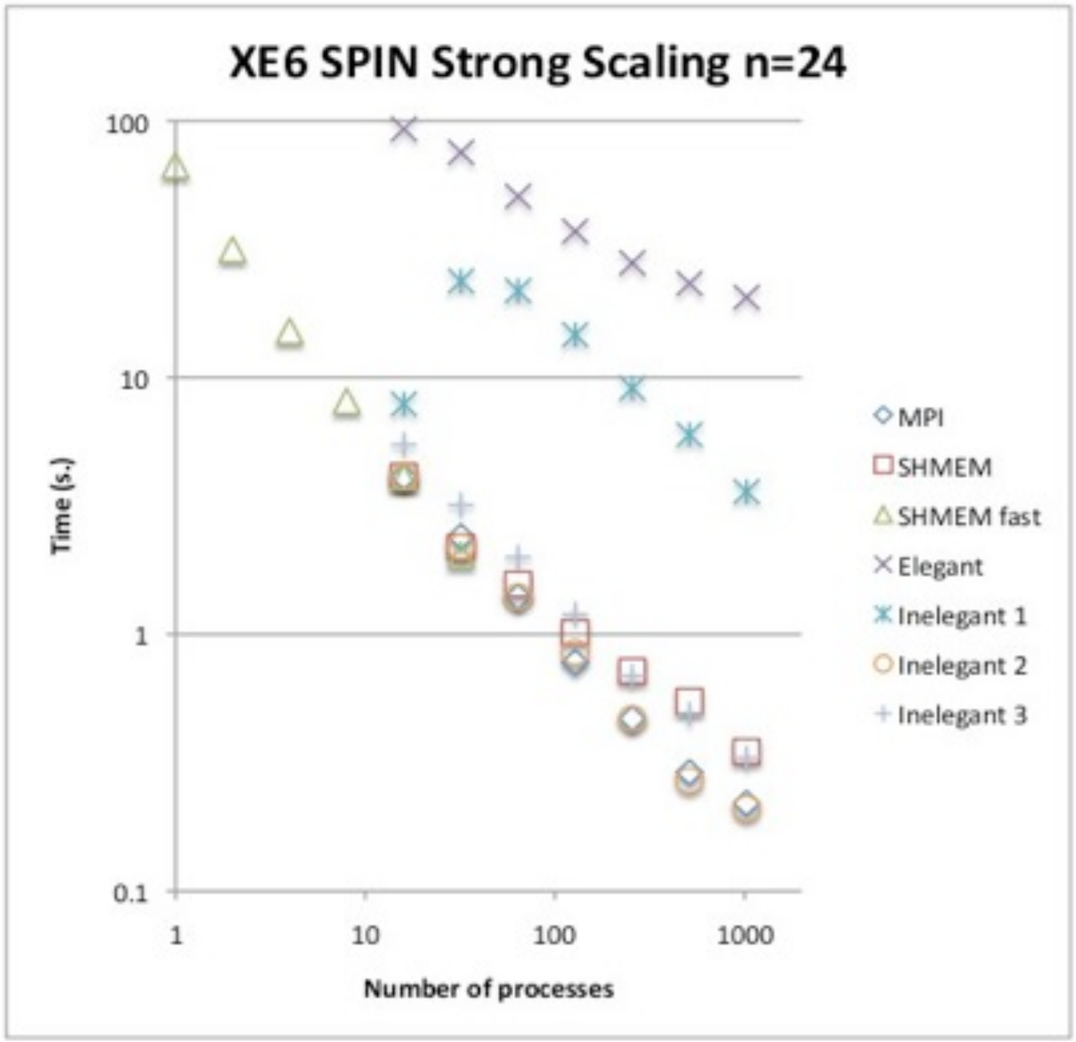

Friday, May 25, 2012

SPIN weak scaling: Cray XE6/Gemini, 10 iterations

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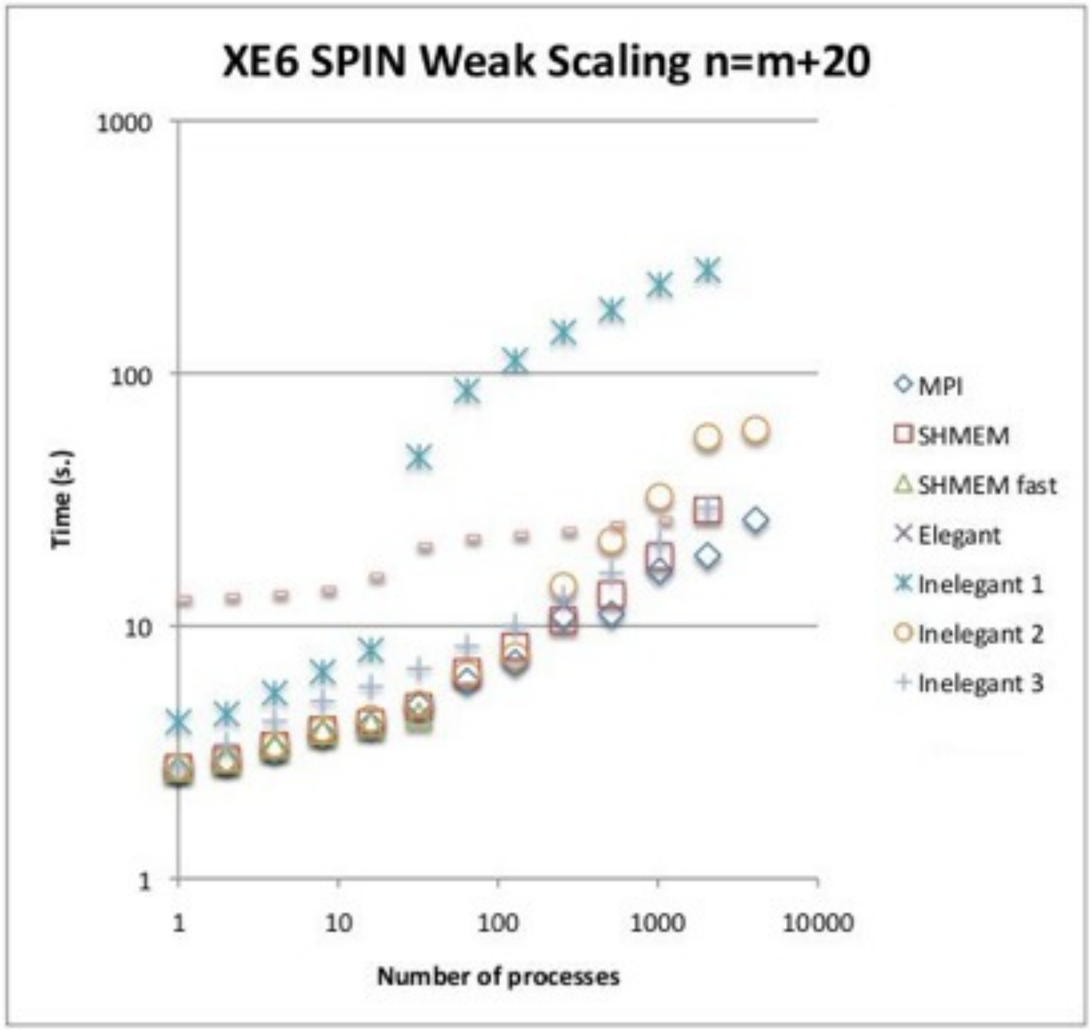

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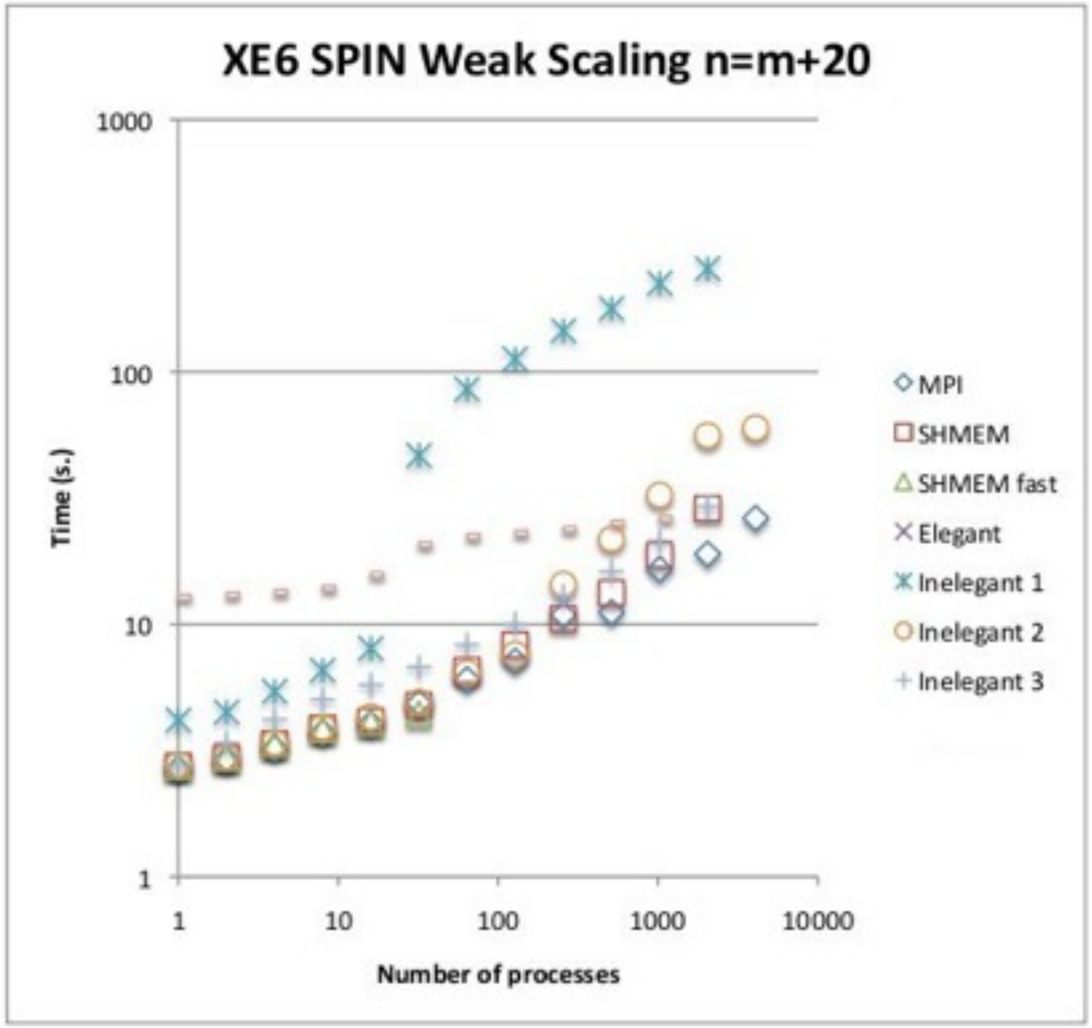

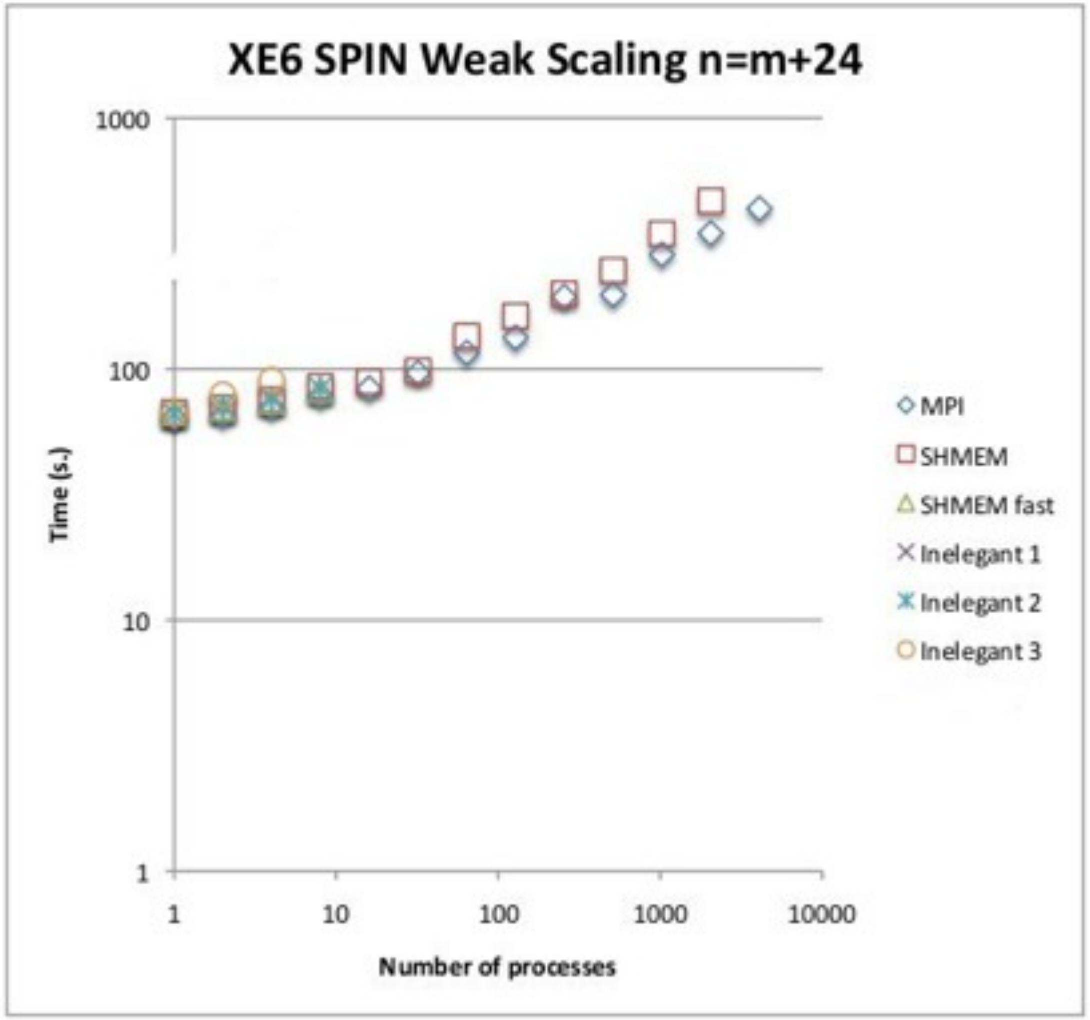

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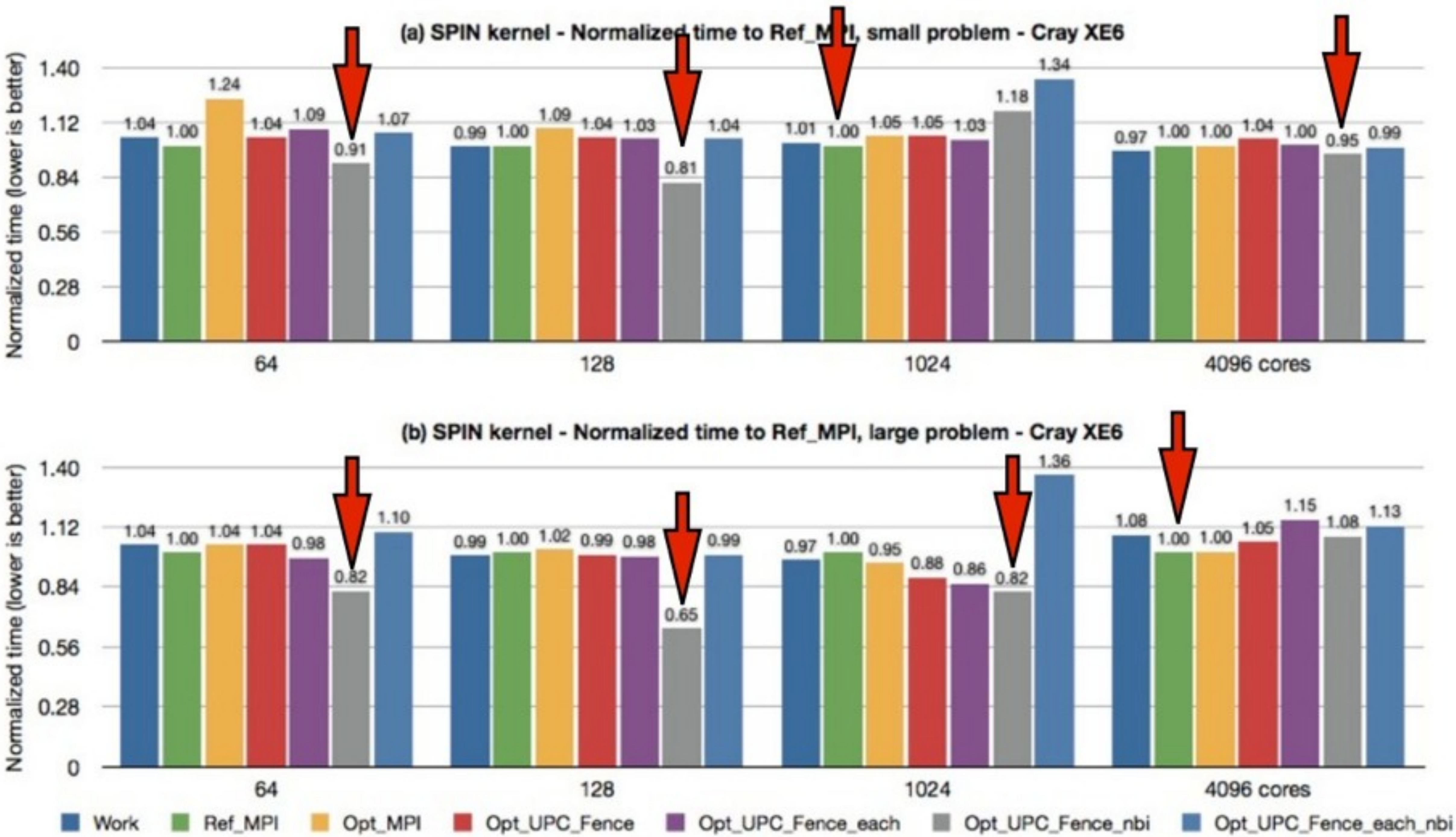

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- PGAS is worthwhile to keep in mind, but
- Currently the investment of changing paradigms does not seem worthwhile

Thank you for your attention!

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