Accelerating the Community Atmosphere Model – Spectral Element Method: The Challenges, the Science, and the Future Direction

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Titan Users and Developers Workshop (East Coast) and Users Meeting
Knoxville, TN
February 19th, 2013

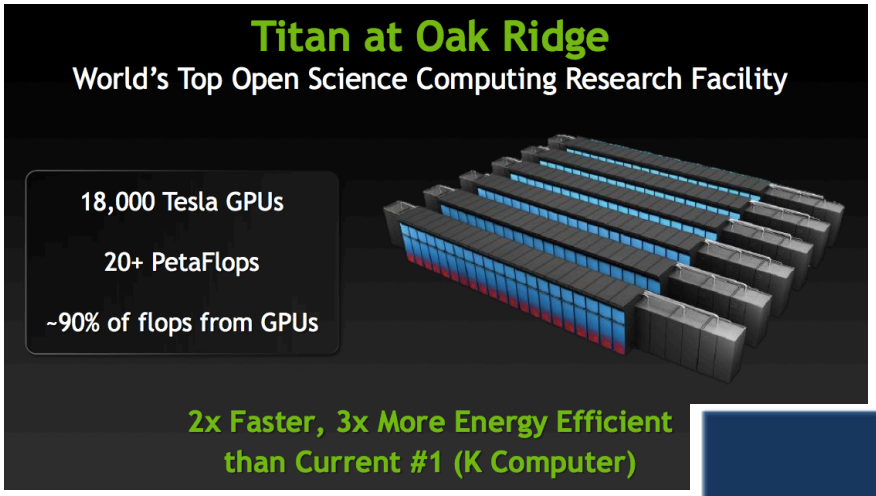
Teams and Projects

Valentine Anantharaj[1,3]	ORNL: OLCF
Rick Archibald[1,2,3]	ORNL: PMG/CCSI
Chris Baker[,2]	ORNL: CEES/CASL
Ilene Carpenter[1]	NREL
Katherine Evans*[23]	ORNL: CESG/CCSI
Jeffrey Larkin[1]	Cray → NVIDIA
Aaron Lott[2]	LLNL
Matthew Norman*[1]	ORNL: OLCF
Paulius Micikevicius[1]	NVIDIA
Mark Taylor[23]	SANDIA
Carrol Woodward[2]	LLNL

***Team/Project Leader**

1. **Center for Accelerated Application Readiness CAM-SE**
2. **Multiscale SCIDAC Process Integration**
3. **Ultra High Resolution Global Climate Simulation**

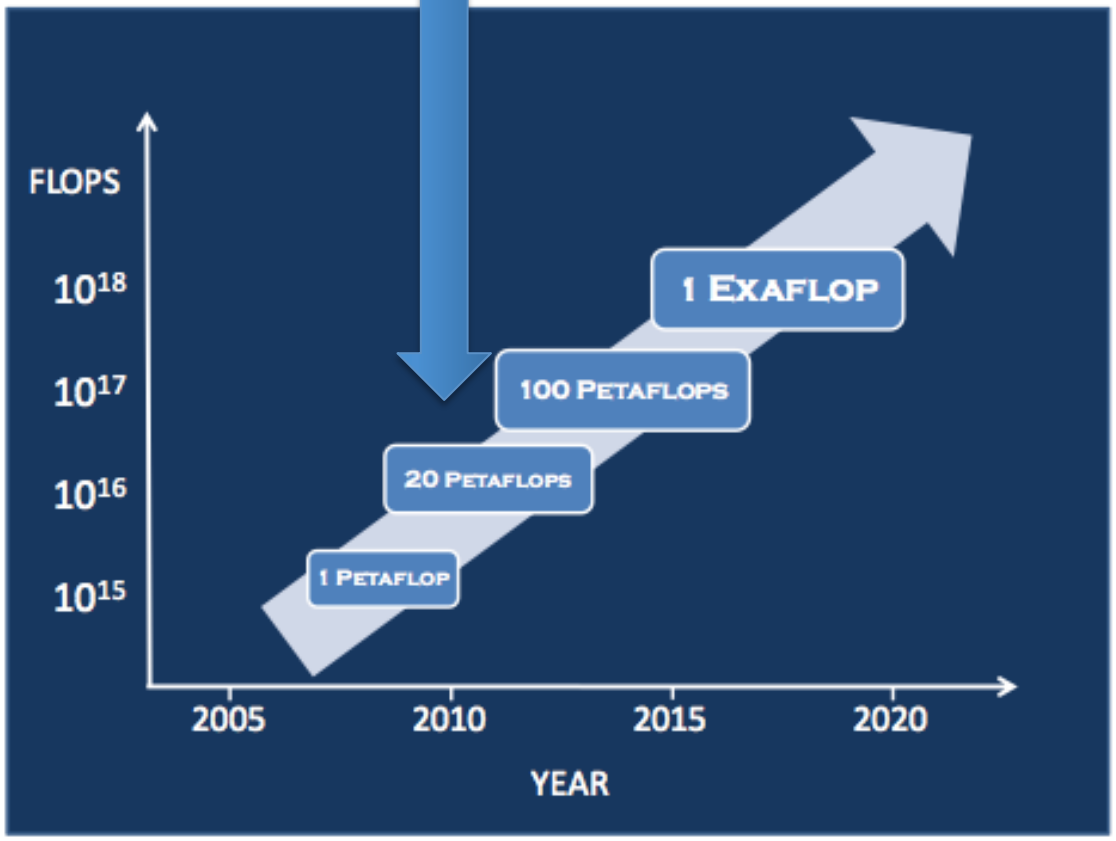
Motivation



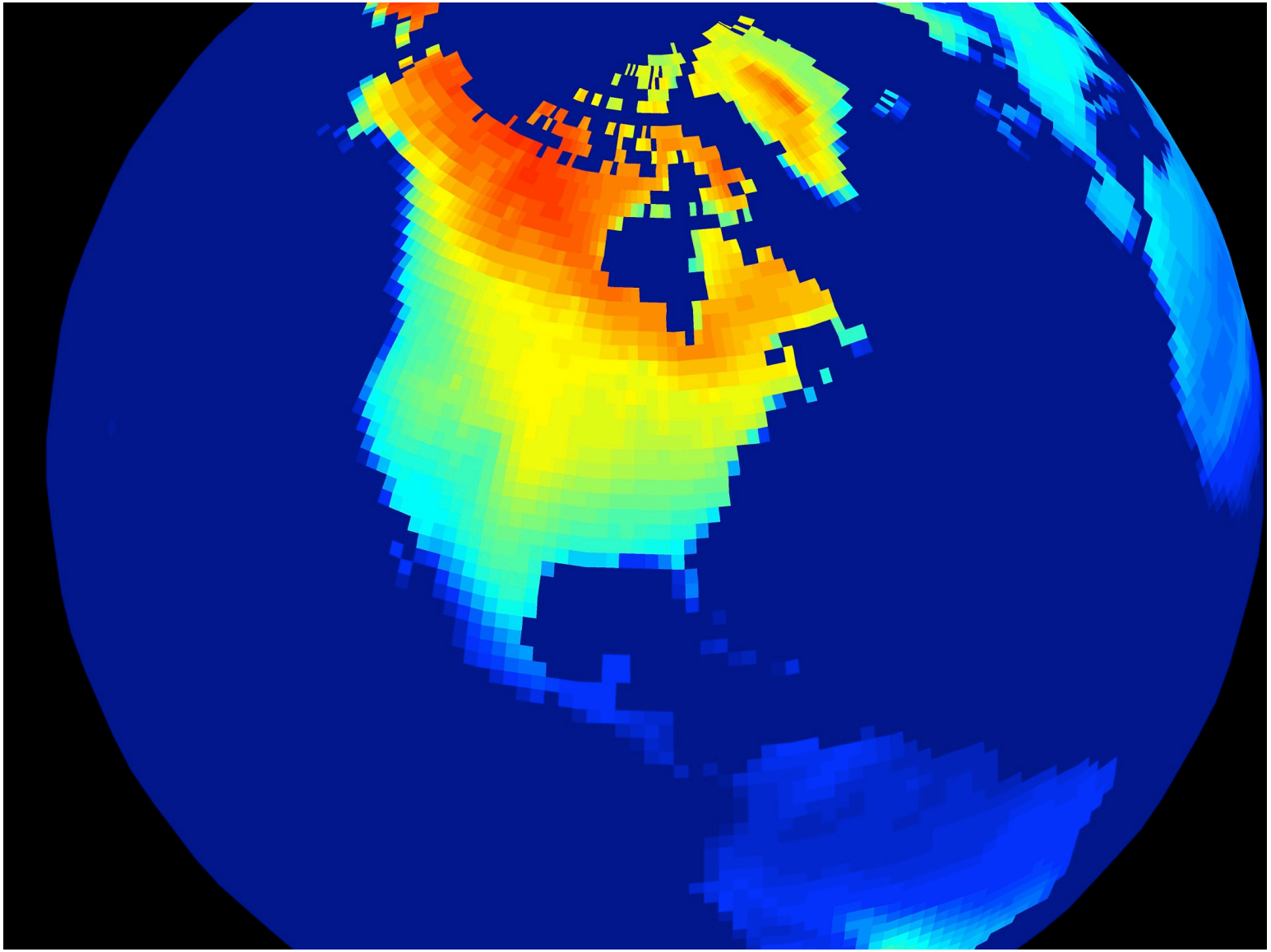
TOP 10 - 06/2012

1	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom
2	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect
3	Mira - BlueGene/Q, Power BQC 16C 1.60GHz, Custom
4	SuperMUC - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR
5	Tianhe-1A - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050
6	Jaguar - Cray XK6, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect,

NVIDIA Update, Jen-Hsun Huang



Motivation: Scientific



Variability of T85 Ensemble over 30 years of Simulation
Global Mean Variation 3 Degrees

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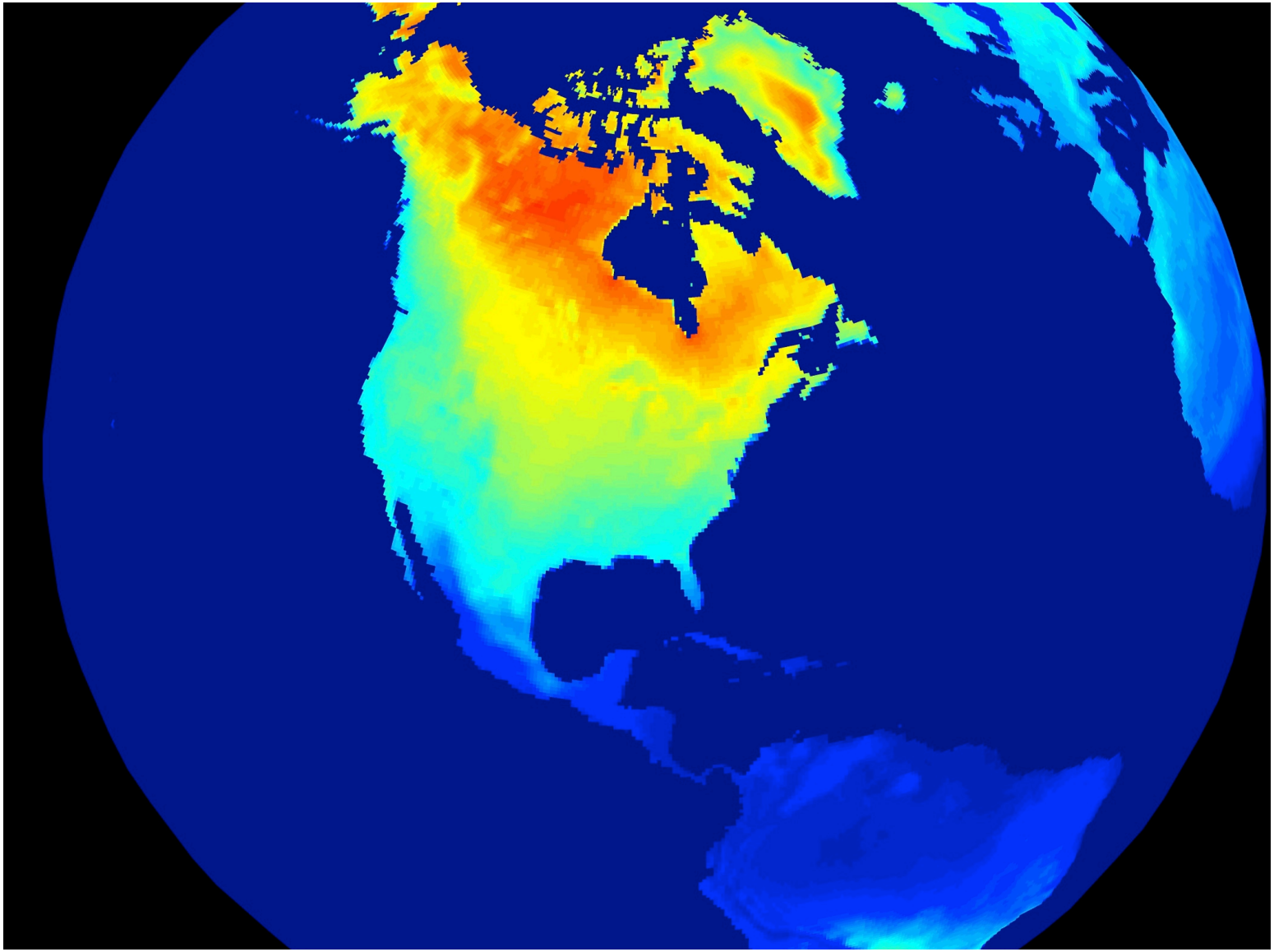
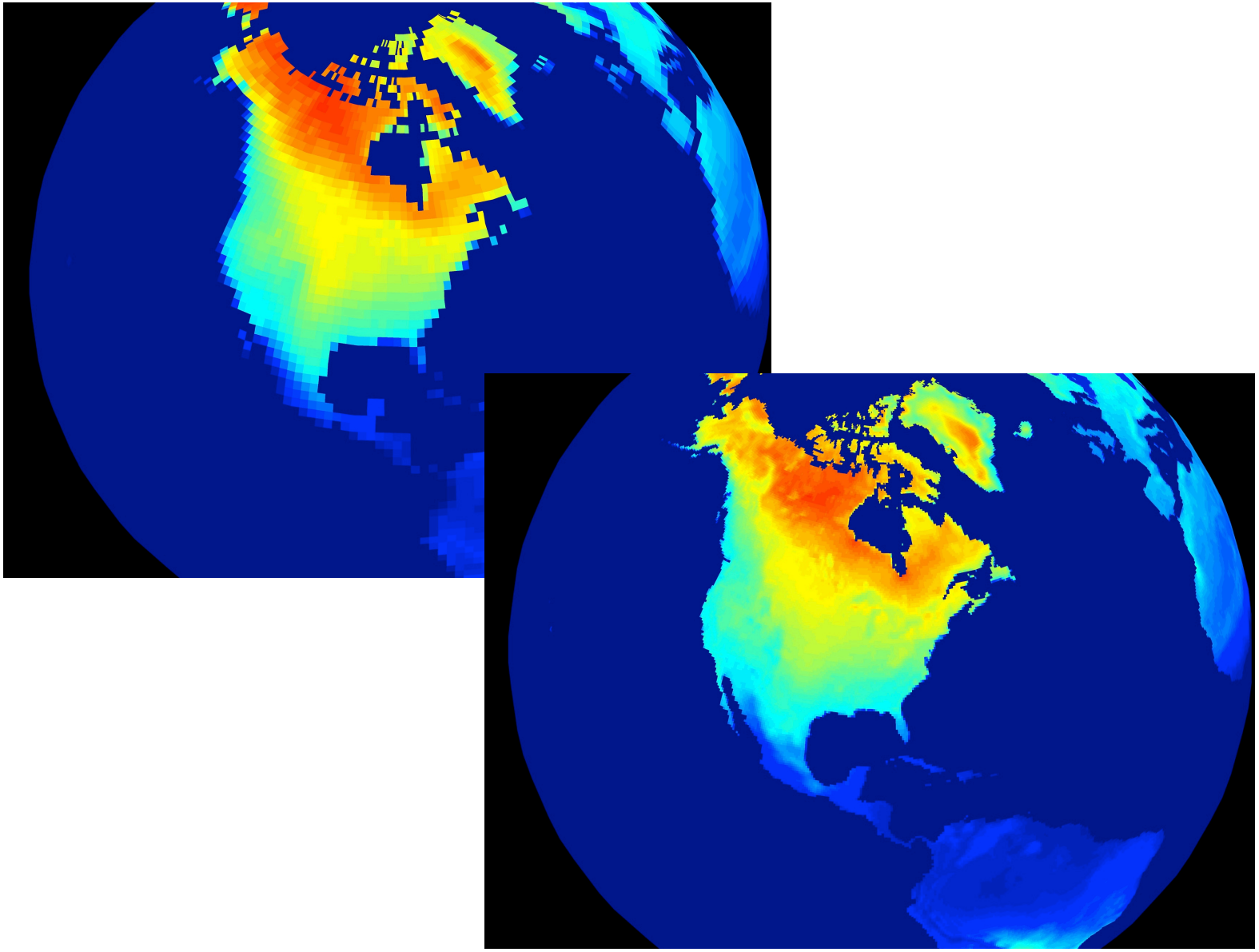


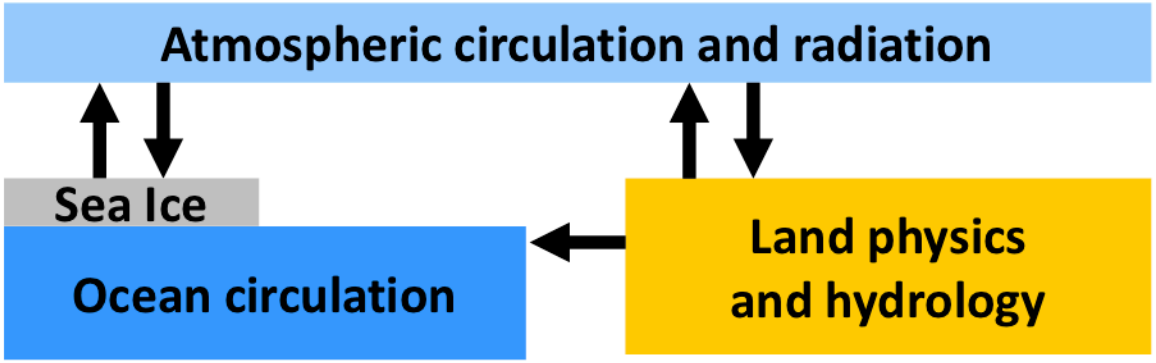
Variability of T341 Ensemble over 30 years of Simulation
Global Mean Variation 3.5 Degrees

Comparison

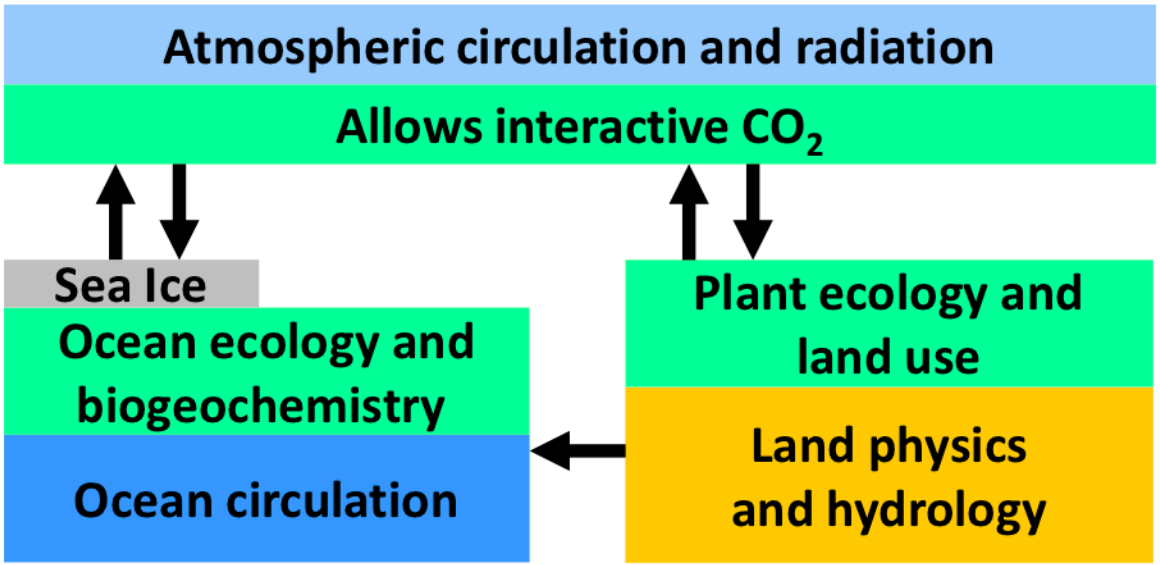


Earth System Model Description

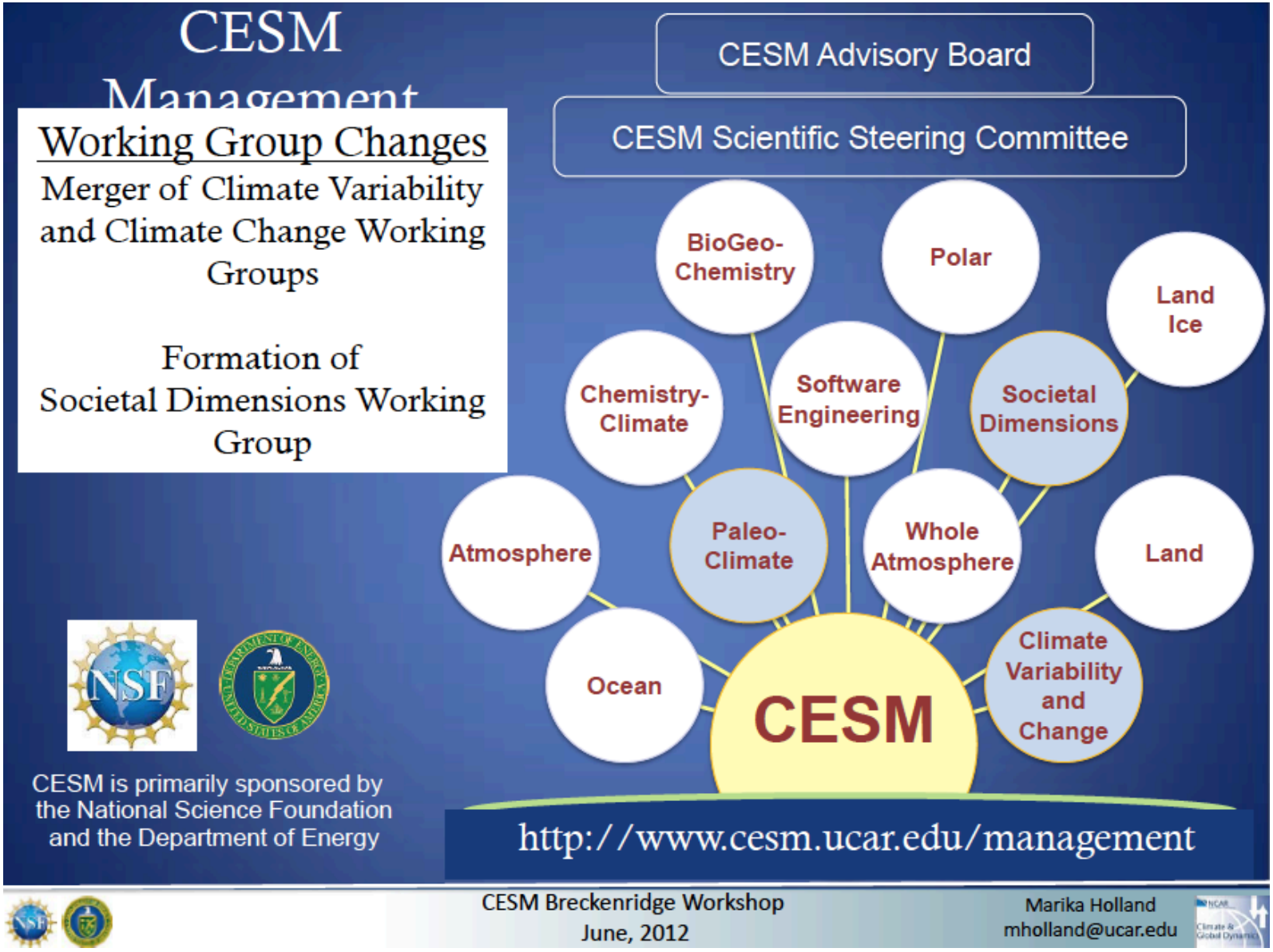
A Climate Model closes the radiative and hydrologic cycles



An Earth System Model closes additional cycles as well



State of the CESM



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- Comprised of (1) a dynamical core and (2) physics packages

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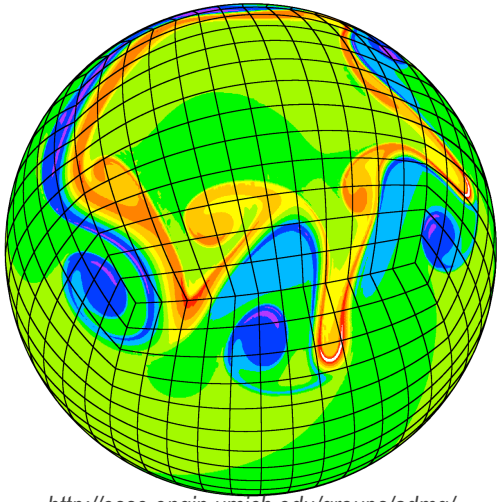

http://esse.engin.umich.edu/groups/admg/dcmip/jablonowski_cubed_sphere_vorticity.png

Dynamical Core

1. "Dynamics": wind, energy, & mass
2. "Tracer" Transport: (H_2O, CO_2, O_3, …)
   Transport quantities not advanced by the dynamics

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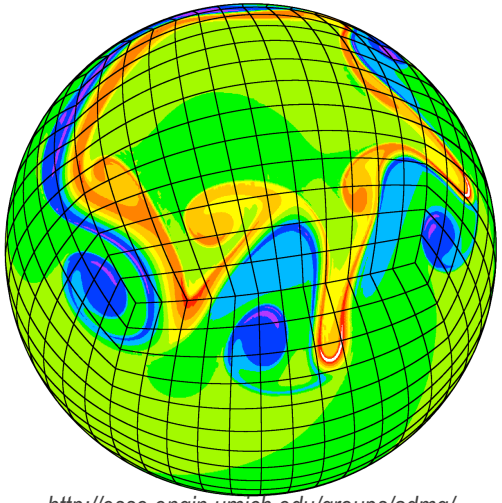

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Dynamical Core

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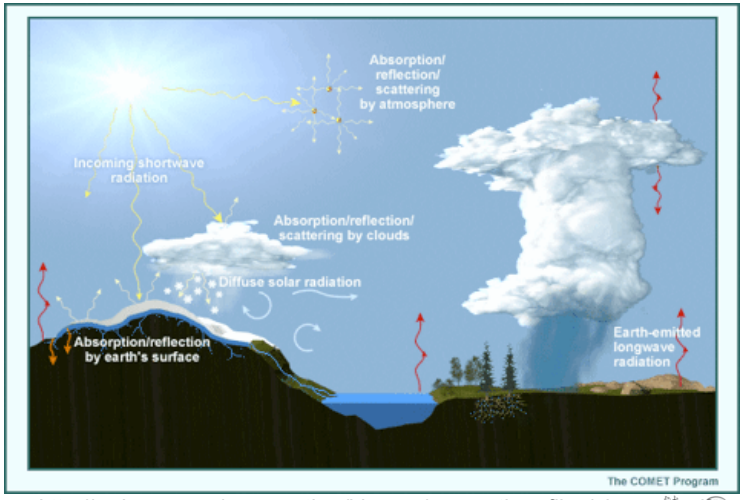
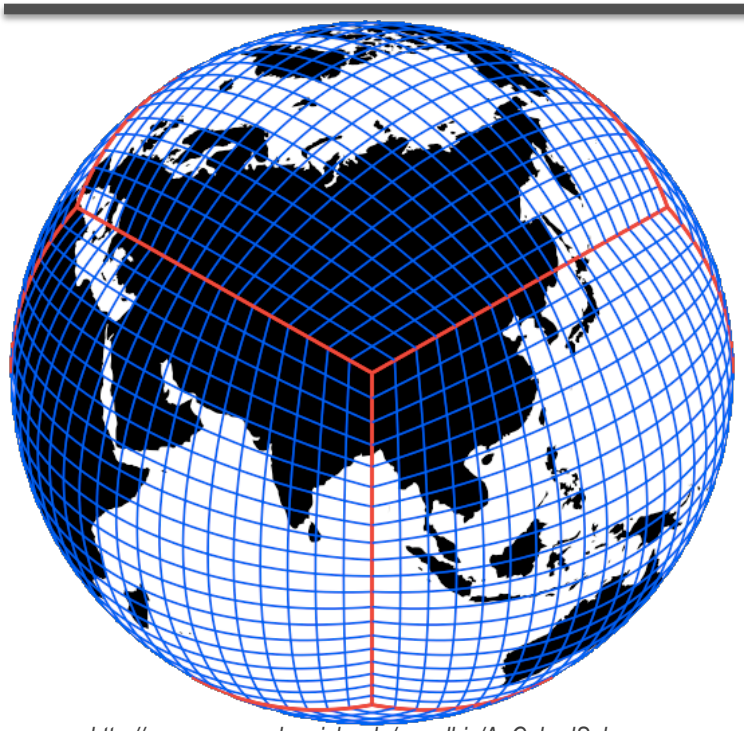
Physics Packages

Resolve anything interesting not included in dynamical core (moist convection, radiation, chemistry, etc)



http://web.me.com/macweather/blogger/maweather_files/physprc2.gif

Gridding, Numerics, & Target Run



http://www-personal.umich.edu/~paullric/A_CubedSphere.png

- Cubed-Sphere + Spectral Element
- Each cube panel divided into elements

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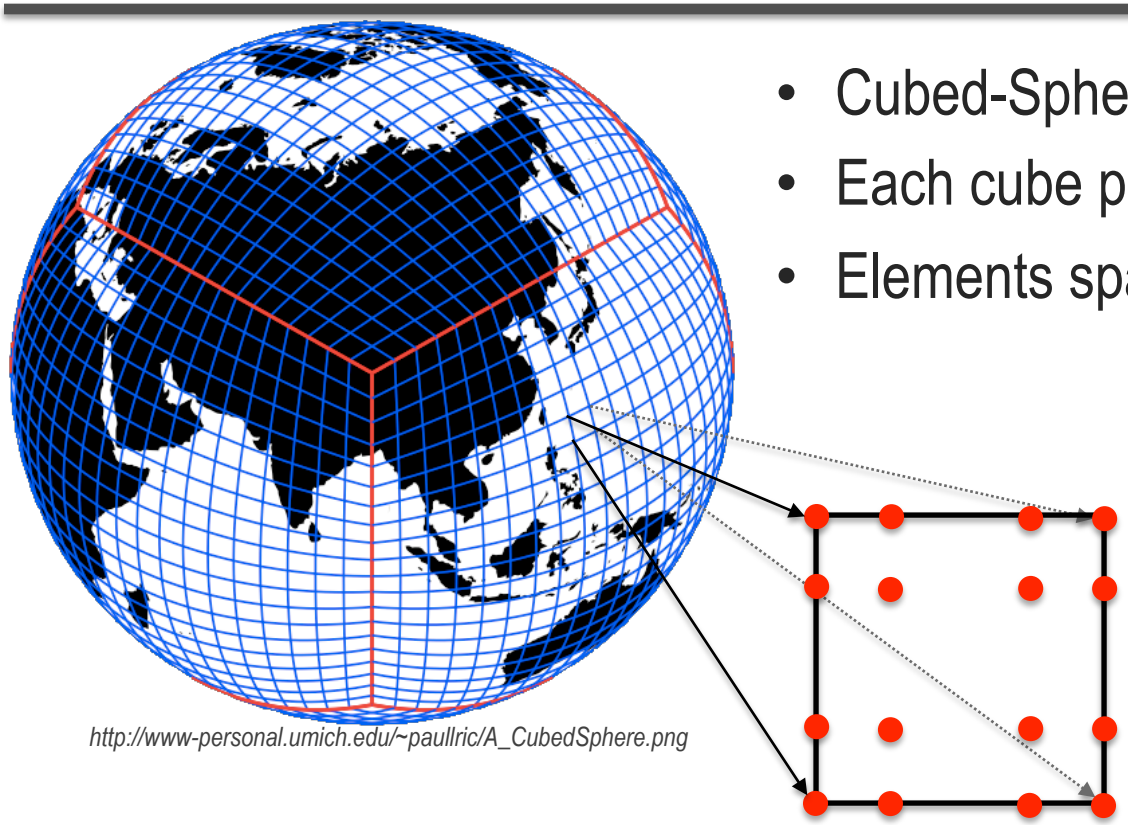

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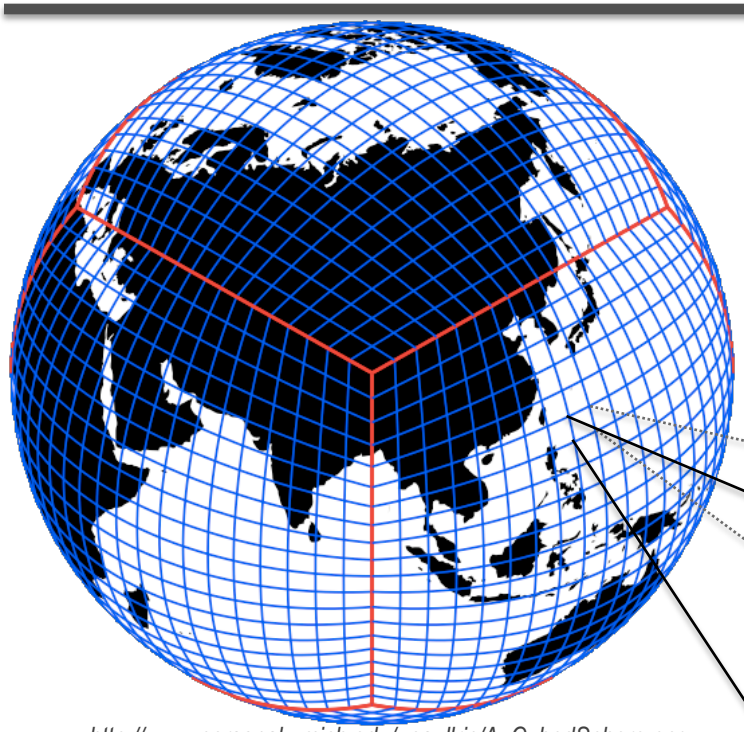

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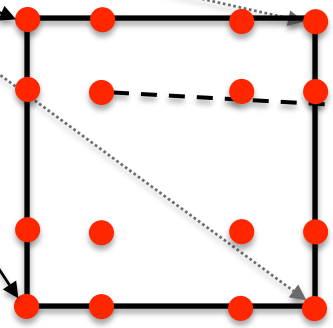
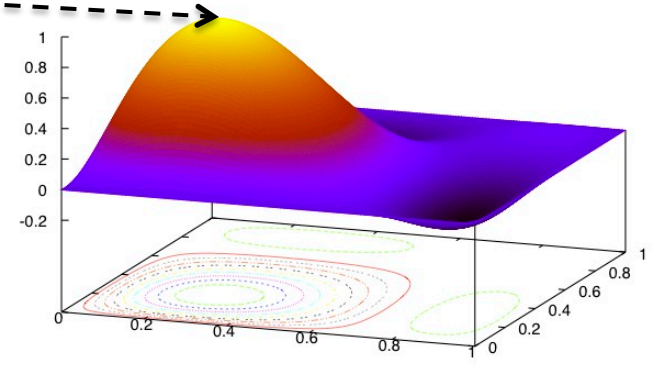
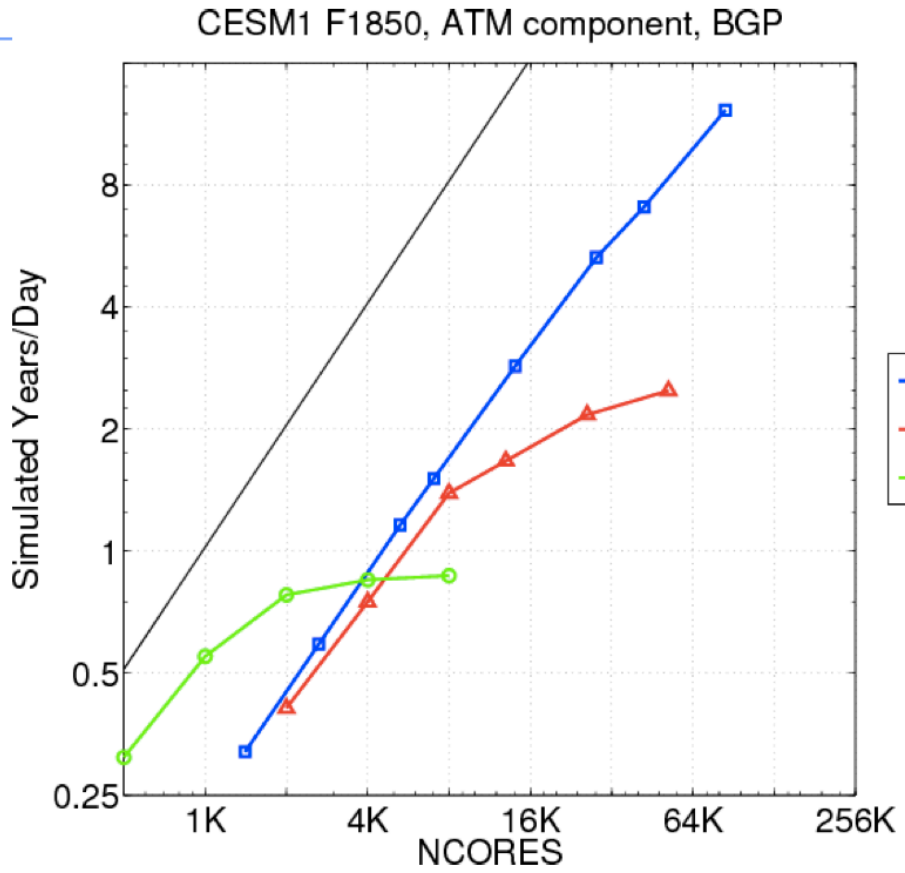
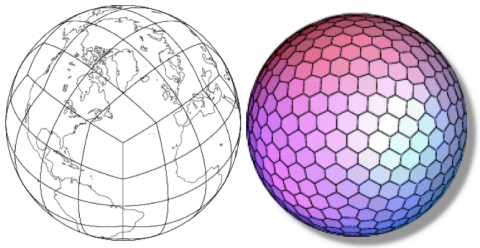
- Cubed-Sphere + Spectral Element
- Each cube panel divided into elements
- Elements spanned by basis functions
- Basis coefficients describe the fluid





Scalability: CAM4 ¼ degree (3 tracers)





- Faster performance at high resolution on parallel computers
- Not cheaper - cost in terms of core-hours is the same.
- CAM-Eul the most efficient (cheapest), but with lowest peak SYPD.

'New capabilities and new dynamical cores in CAM'. Mark Taylor, 16th Annual CESM Workshop, 2011.

Target 14km Simulations

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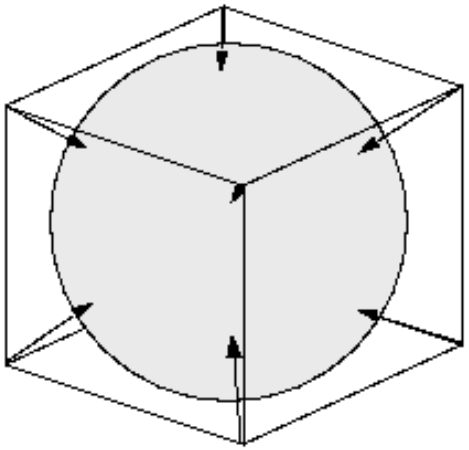

Target 14km Simulations

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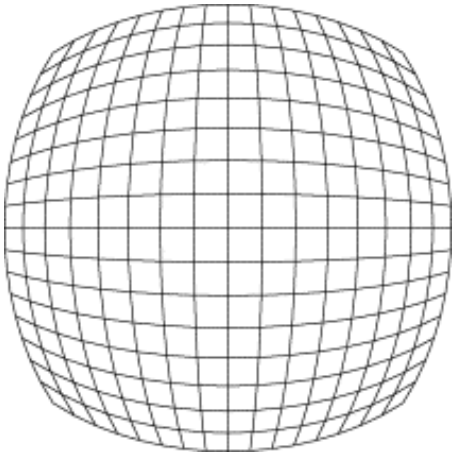

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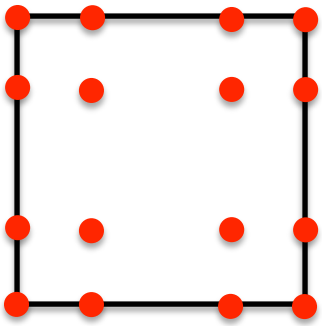
  - 240 x 240 columns of elements per panel
  - 4 x 4 basis functions per element



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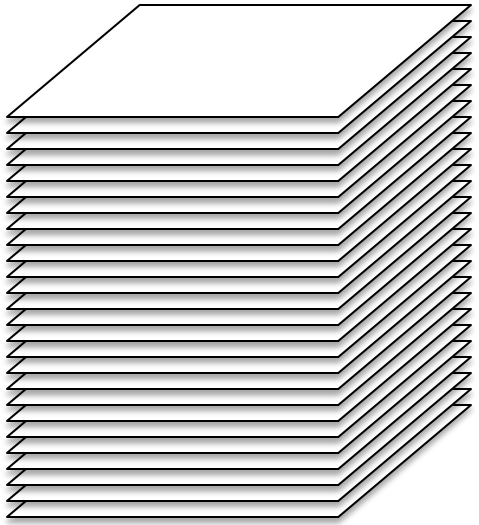
  - 26 vertical levels



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  - 110 prognostic variables

$$\rho, \rho u, \rho v, p$$

$$H_2O \ , \ CO_2 \ , \ O_3 \ , \ CH_4 \ , \ ...$$

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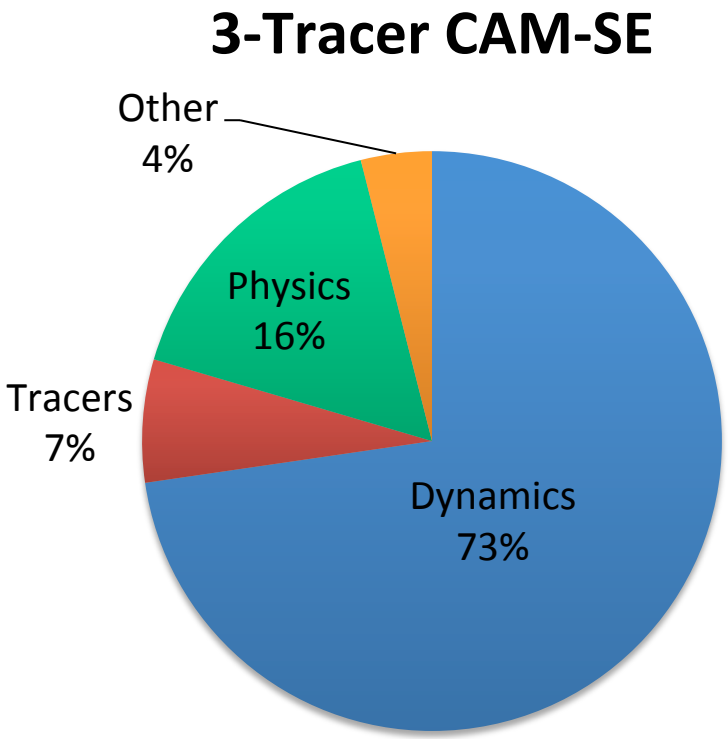
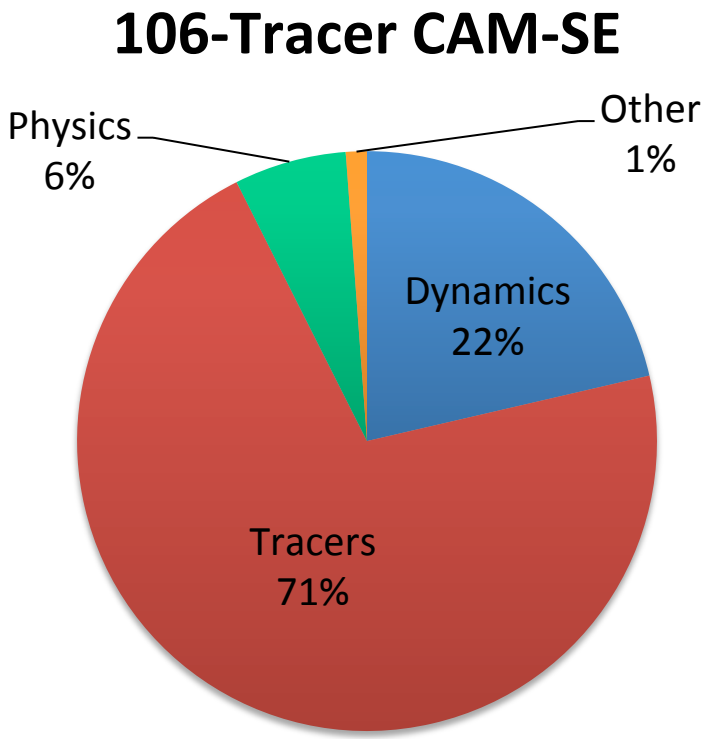
- Scaled to 14,400 XT5 nodes with 60% parallel efficiency
- Must simulate 1-2 thousand times faster than real time
- With 10 second CAM-SE time step, need ≤ 10 ms per time step
  - 32-64 columns of elements per node, 5-10 thousand nodes

CAM-SE Profile (Cray XT5, 14K Nodes)

- Original CAM-SE used 3 tracers (20% difficult to port)
- Mozart chemistry provides 106 tracers (7% difficult to port)
  - Centralizes port to tracers with mostly data-parallel routines





The Routines of Tracer Transport

Three Main Routines

- **Euler_step (3x)**: Performs the actual transport
- **Advance_hypervis**: Stabilizes the solution with ∇^4 diffusion
- **Vertical_Remap**: Re-grids the data vertically to a reference grid

Three Helper Routines

- **Edge_pack**: Place all element edges into process-wide buffer
  Edge_unpack: Sum data at element edges
  - *Once* per euler_step *Twice* per advance_hypervis
- **Limiter2d_zero**: Remove negative coefficients & conserve mass
  - *Once* per euler_step *Once* per advance_hypervis

Call Tree Structure

```
prim_main
```

Main driver routines

```
prim_run_subcycle
```

Time stepping routines

```
prim_advec_tracers...
```

Tracer advection routines

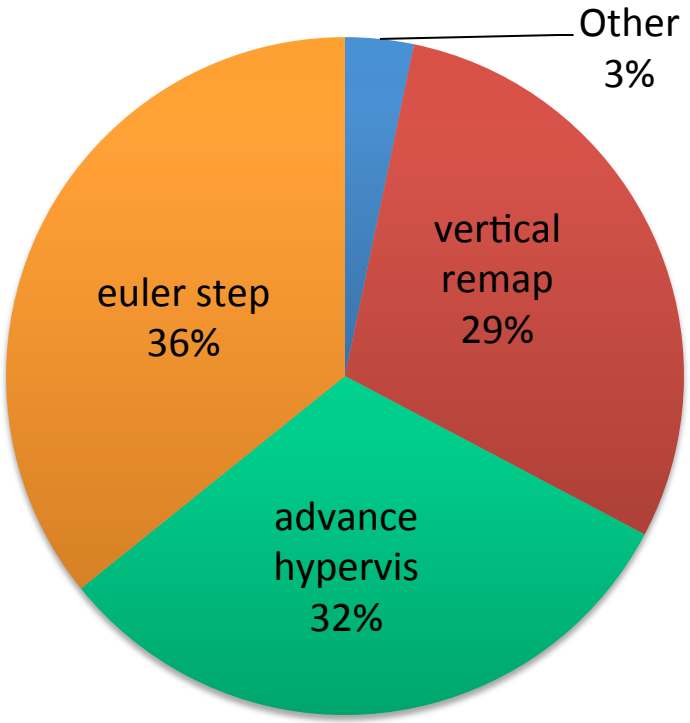
```
euler_step
  edgevpack
  bndry_exchangev   }=pack-unpack
  edgevunpack
    laplace_sphere_wk
      pack-unpack
remap_velocity
```

This routine called multiple times depending upon the type of timestep (ie, leapfrog, RK, etc).

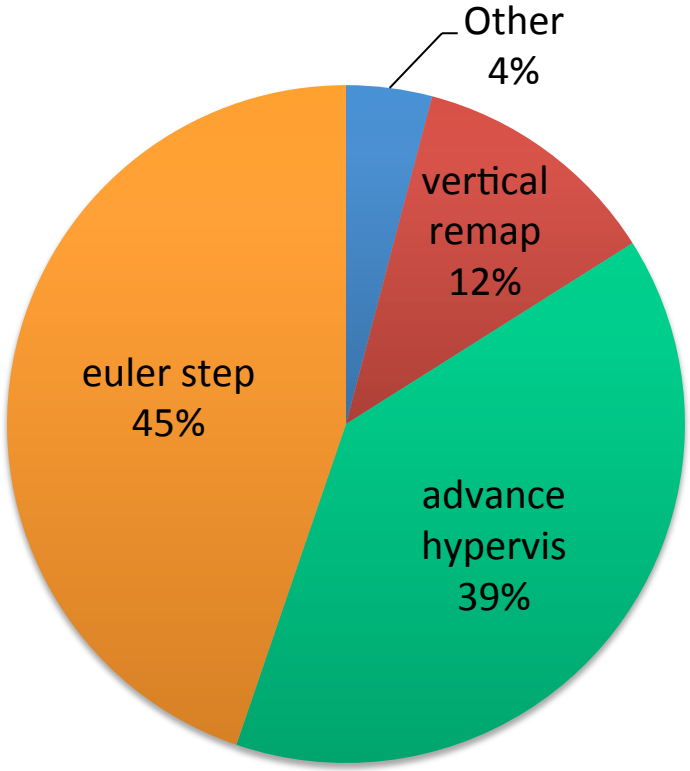
Profile of a Tracer Time Step

- We wrote a new remapping algorithm to reduce runtime
- Pack/exchange/unpack is ≈ half of euler_step & advance_hypervis

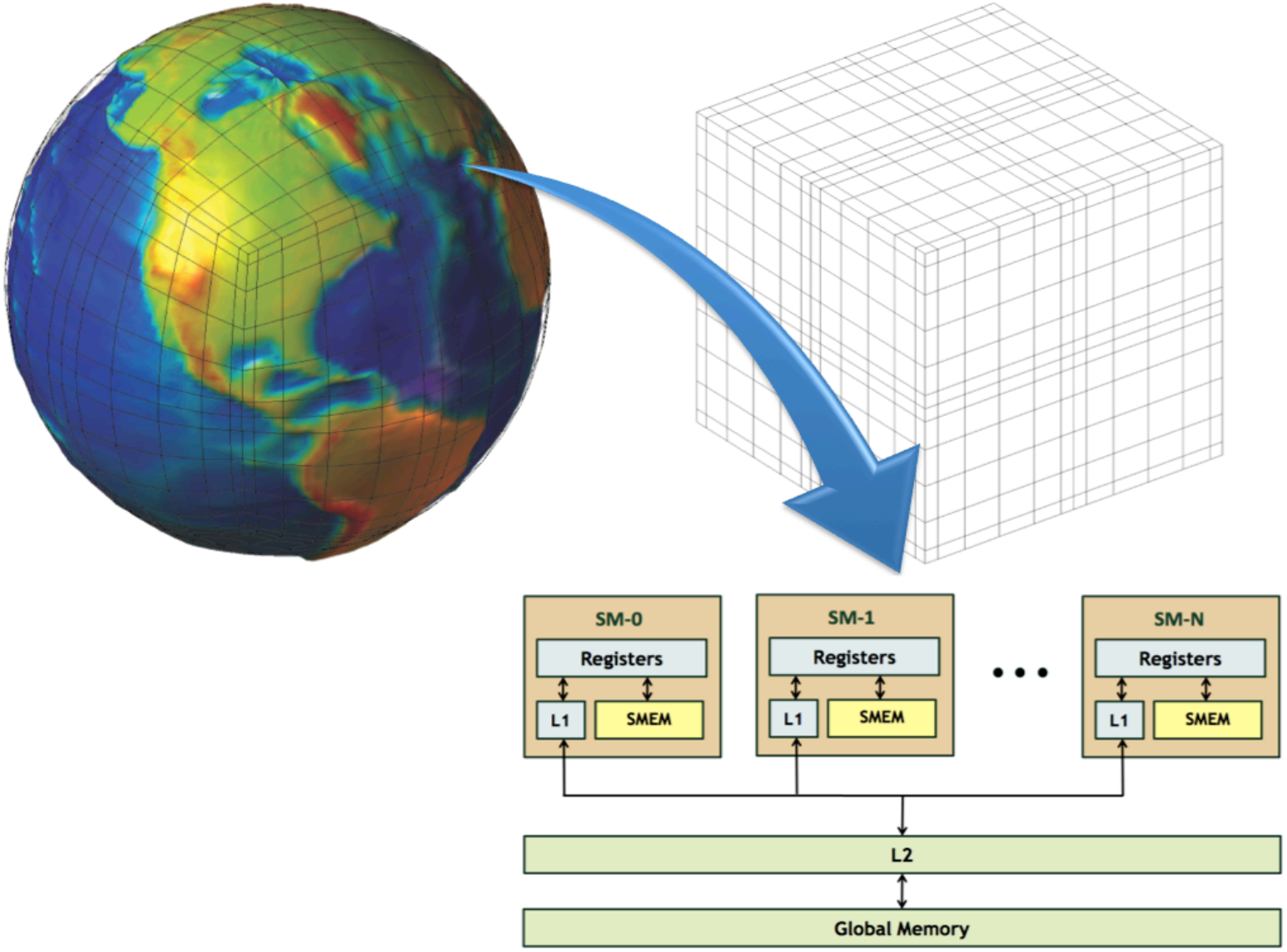
Original Vertical Remap



New Vertical Remap



GPU CAM-SE Goal



Node Design

http://www.thinkdigit.com/FCKeditor/uploads/26mar10470oin342t.jpg

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GPU Kernels


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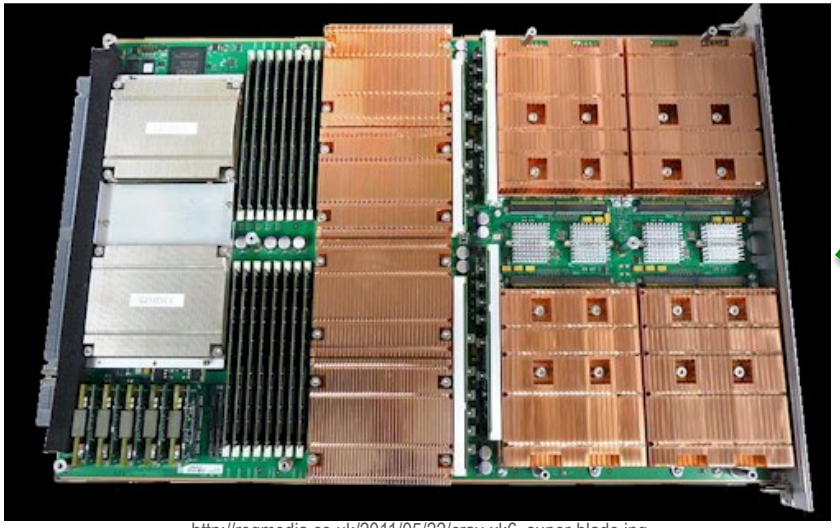
PCI-e D2H



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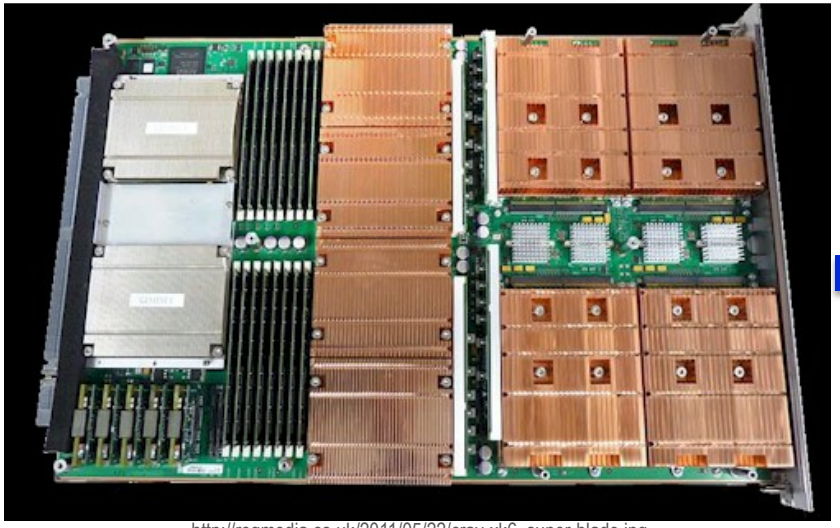

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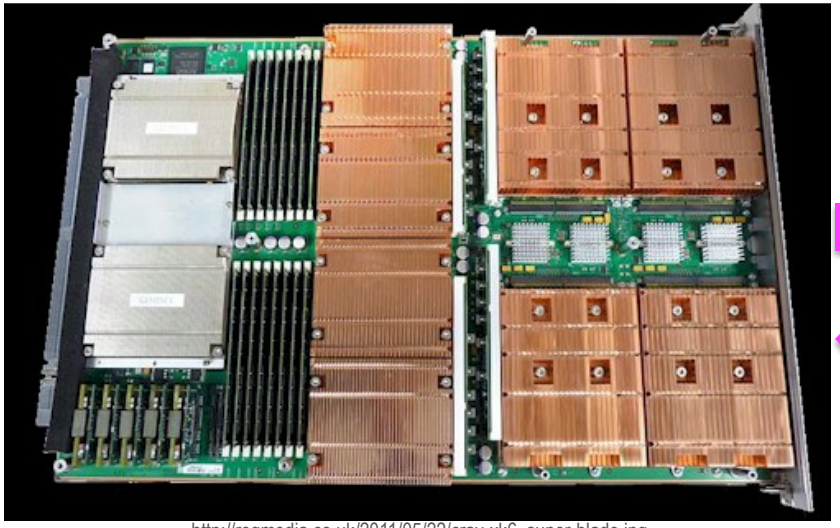
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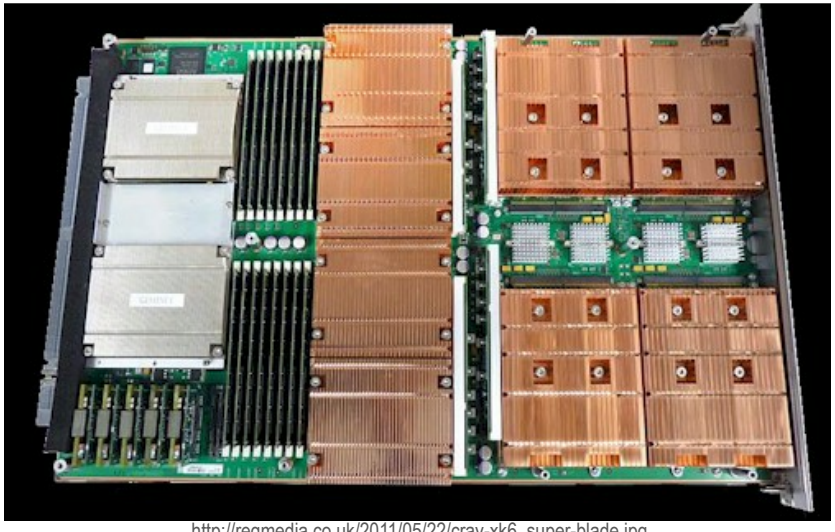
Host Computation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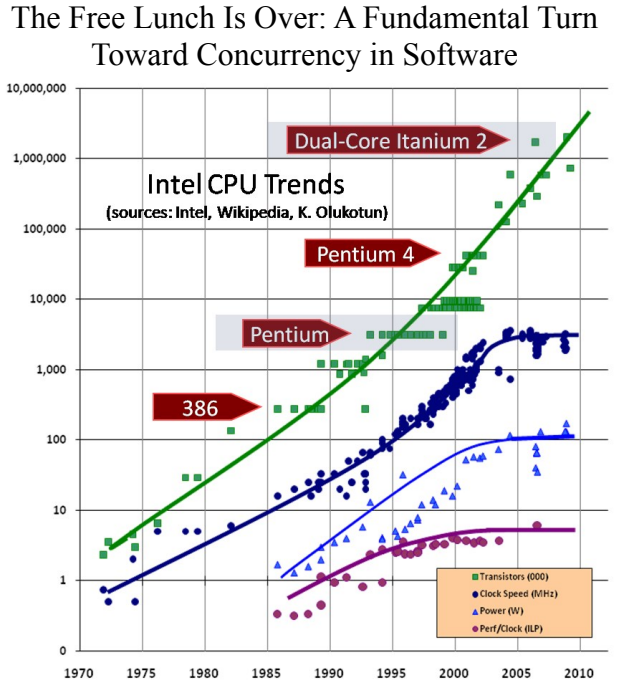

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If you were plowing a field, which would you rather use: 2 strong oxen or 1024 chickens?

– Seymour Cray

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If you were plowing a field, which would you rather use: 12,160 bipolar oxen[1] or 786,432 chickens[2]?

– Not Seymour Cray

http://regmedia.co.uk/2011/05/22/cray-xk6_super-blade.jpg

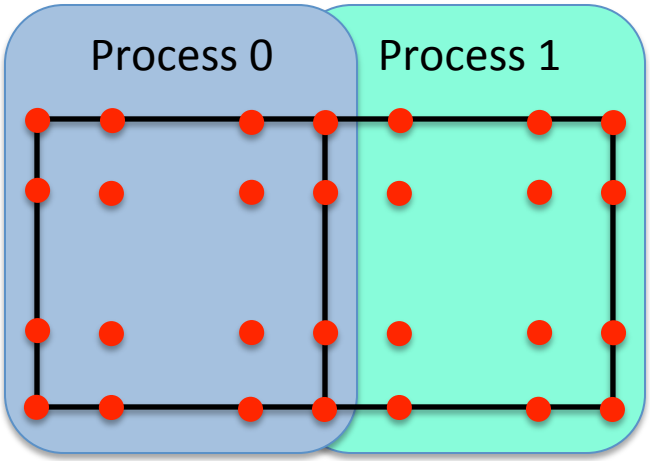
[1] A bipolar oxen is one AMD Bulldozer and one NVIDIA Fermi.
[2] A chicken is a Blue Gene/Q core.

Herding millions of chickens: Programming models for Blue Gene/Q and beyond

Jeff Hammond

Leadership Computing Facility
Argonne National Laboratory

Communication Between Elements



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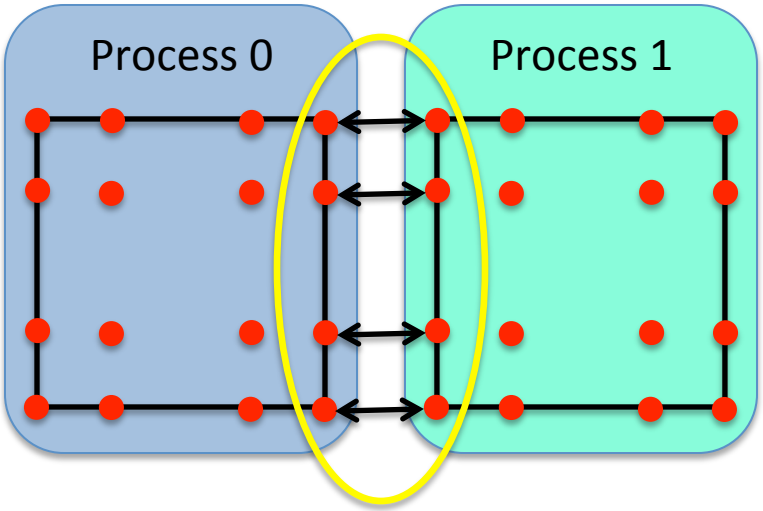

Physically occupy the same location, Spectral Element requires them to be equal

Edges are averaged, and the average replaces both edges

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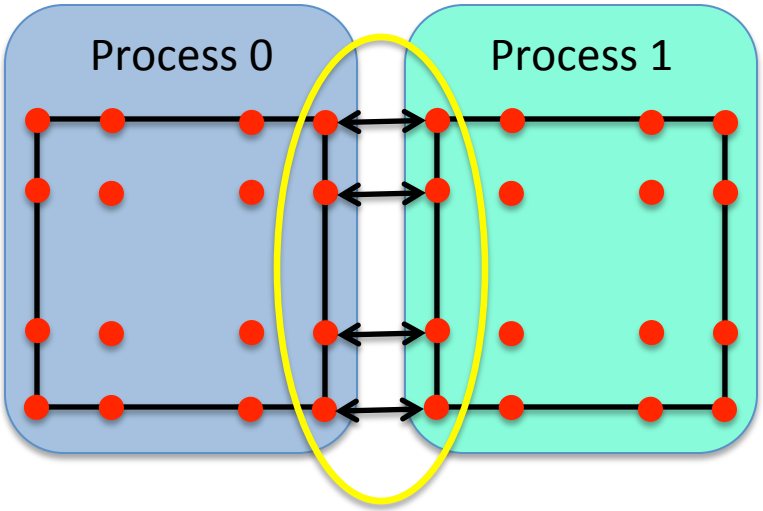

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Edges are averaged, and the average replaces both edges

Implementation

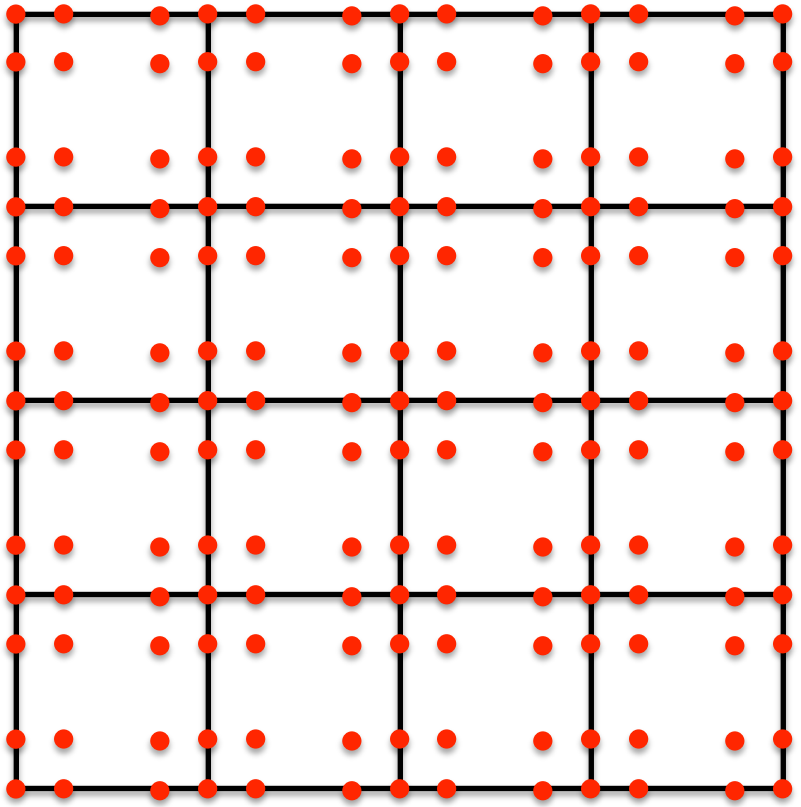
Edge_pack: pack all element edges into process-wide buffer. Data sent over MPI are contiguous in buffer.

Bndry_exchange: Send & receive data at domain decomposition boundaries

Edge_unpack: Perform a weighted sum for data at all element edges.

Original Pack/Exchange/Unpack

- Edge_pack ensures data for MPI is contiguous in buffer
- MPI communication occurs in “cycles”



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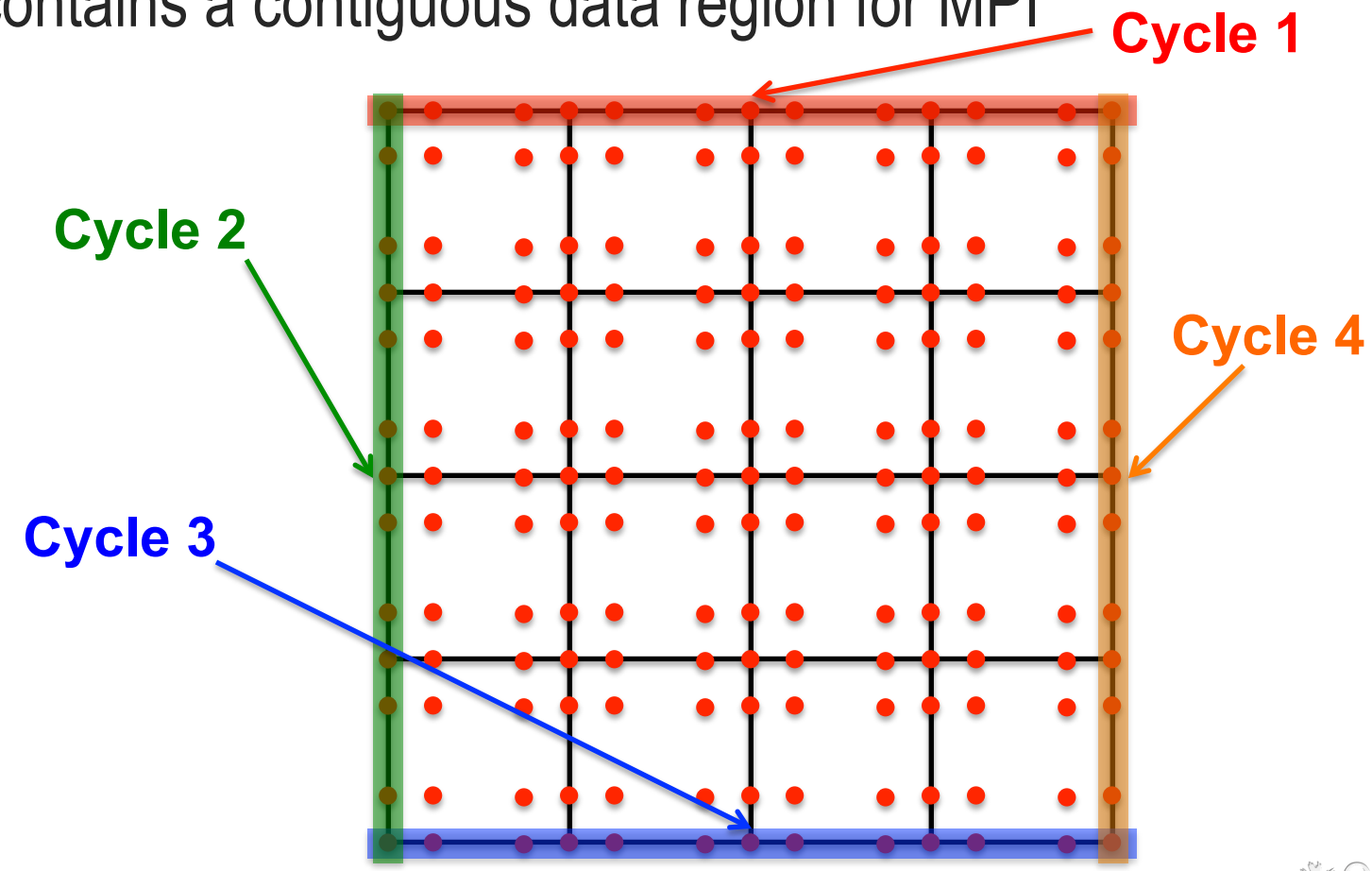

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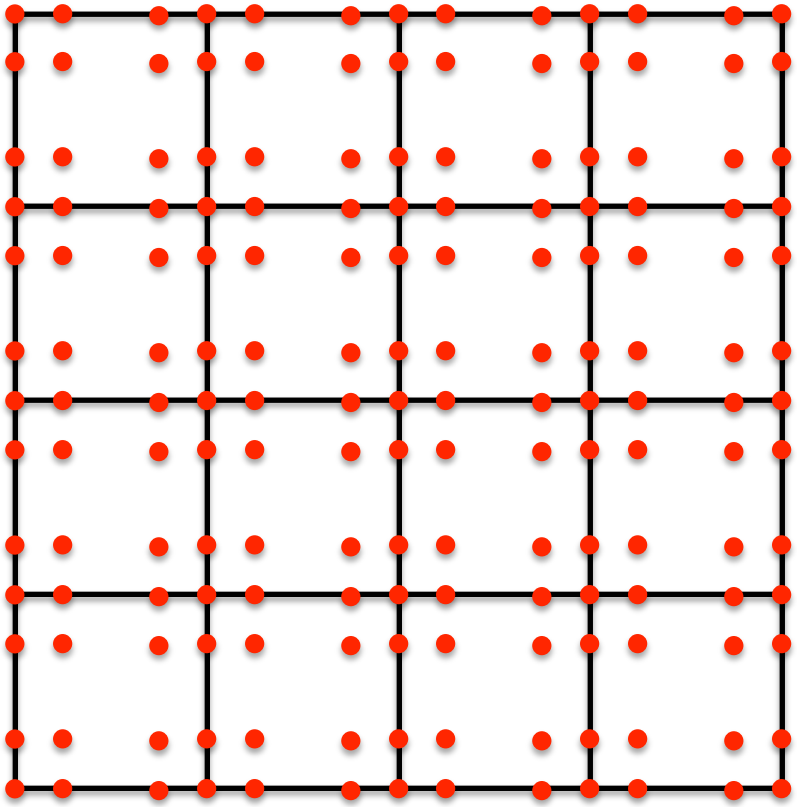

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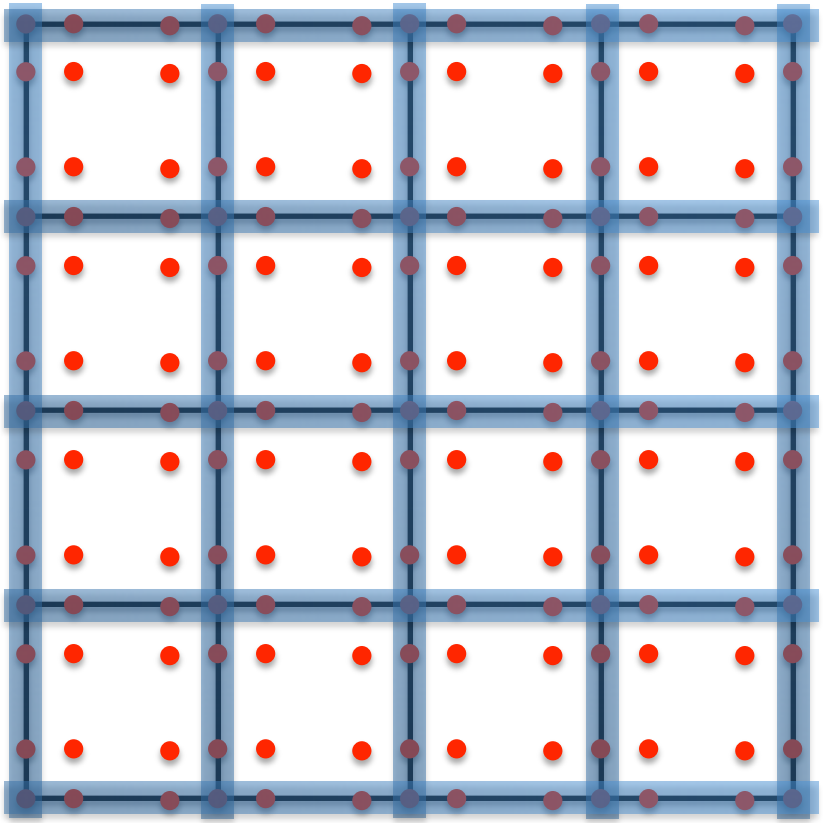

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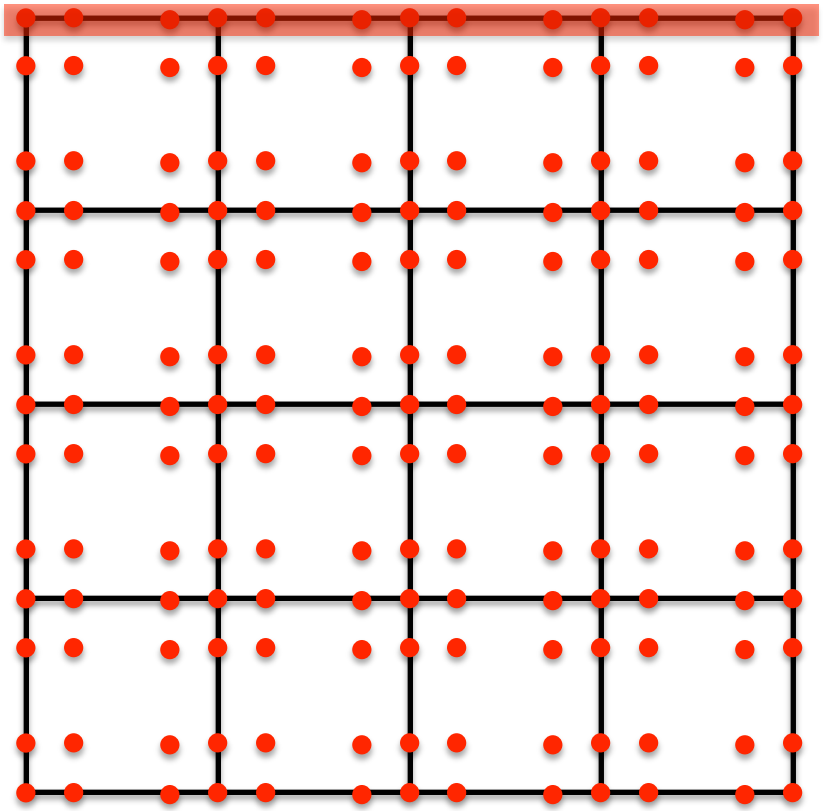

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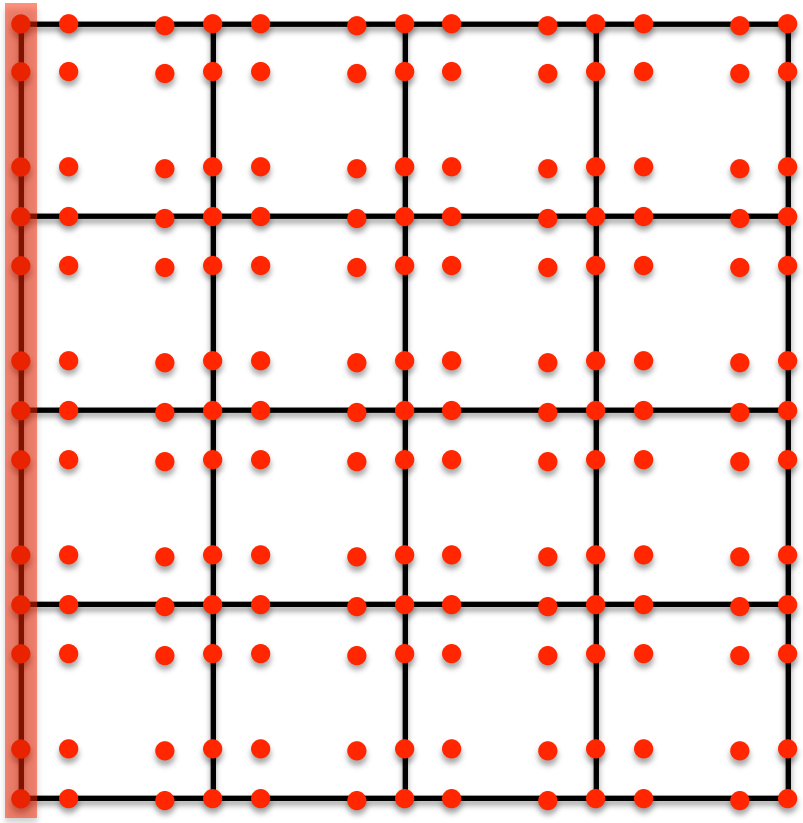

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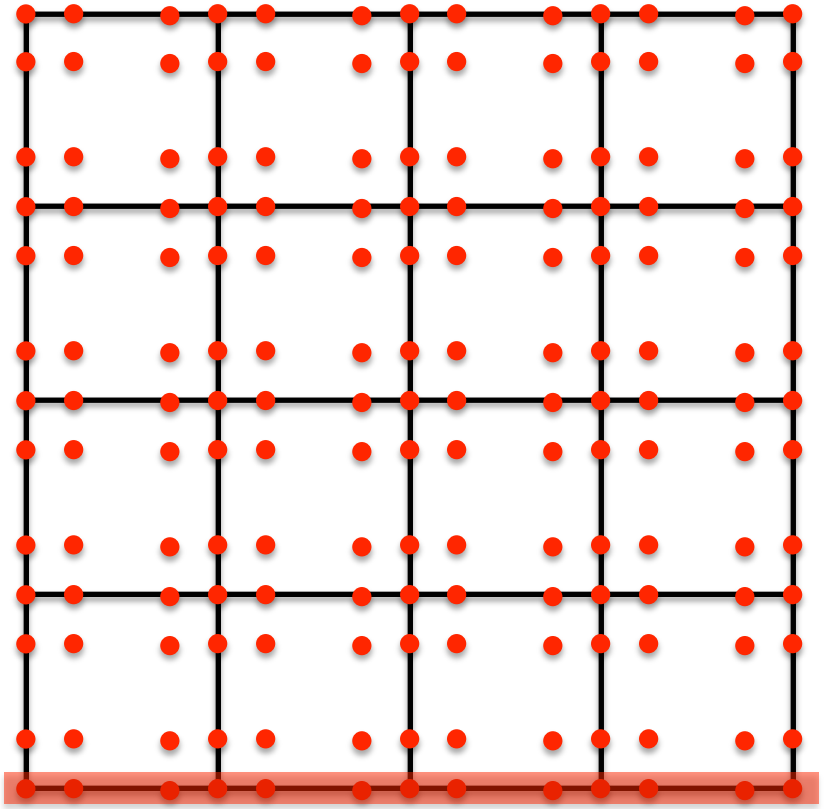

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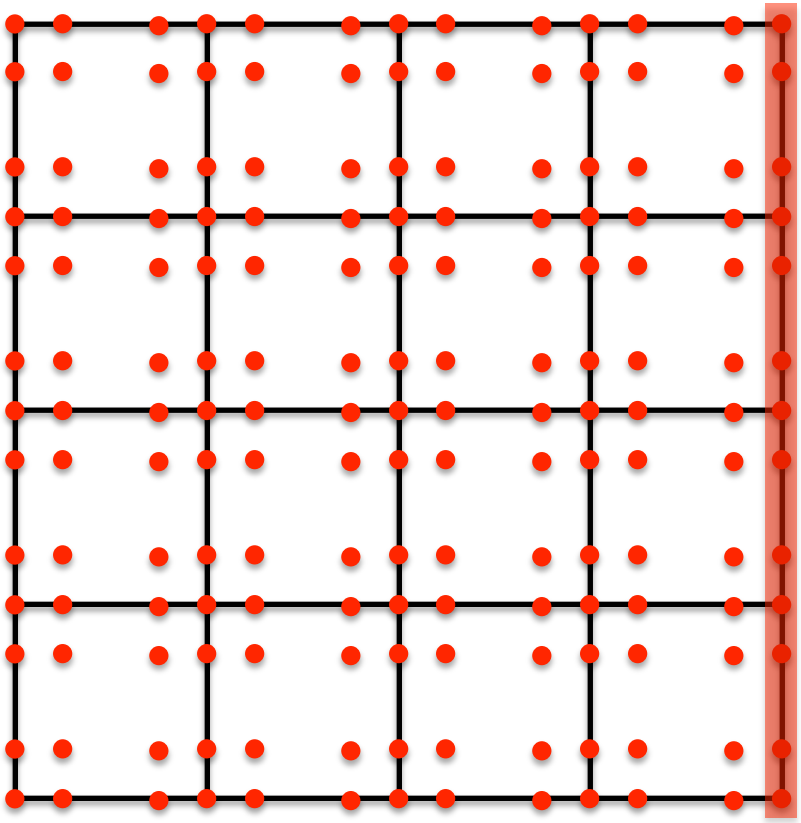

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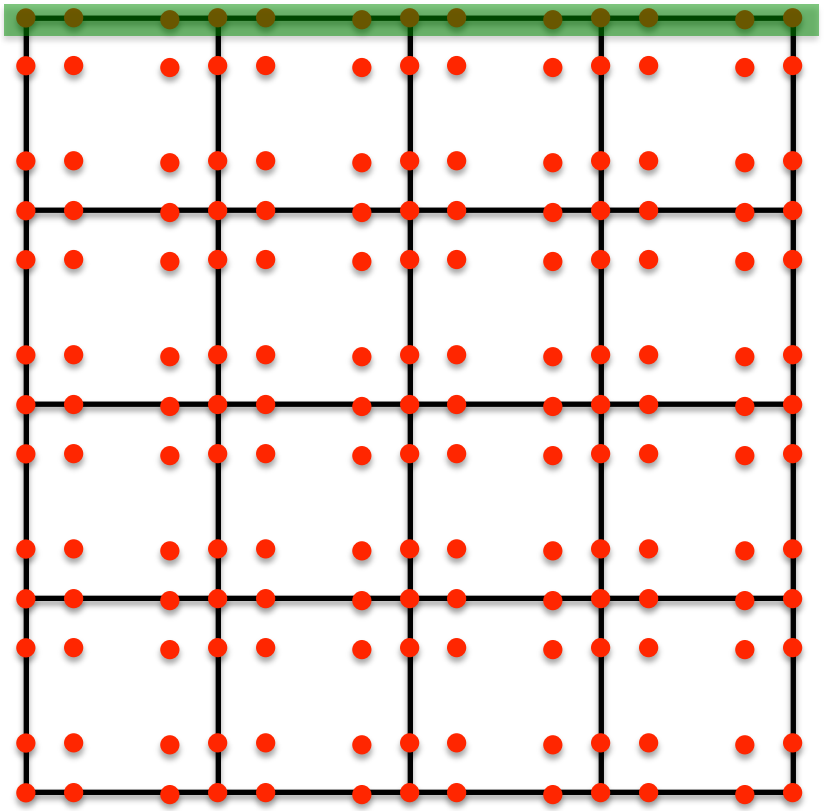

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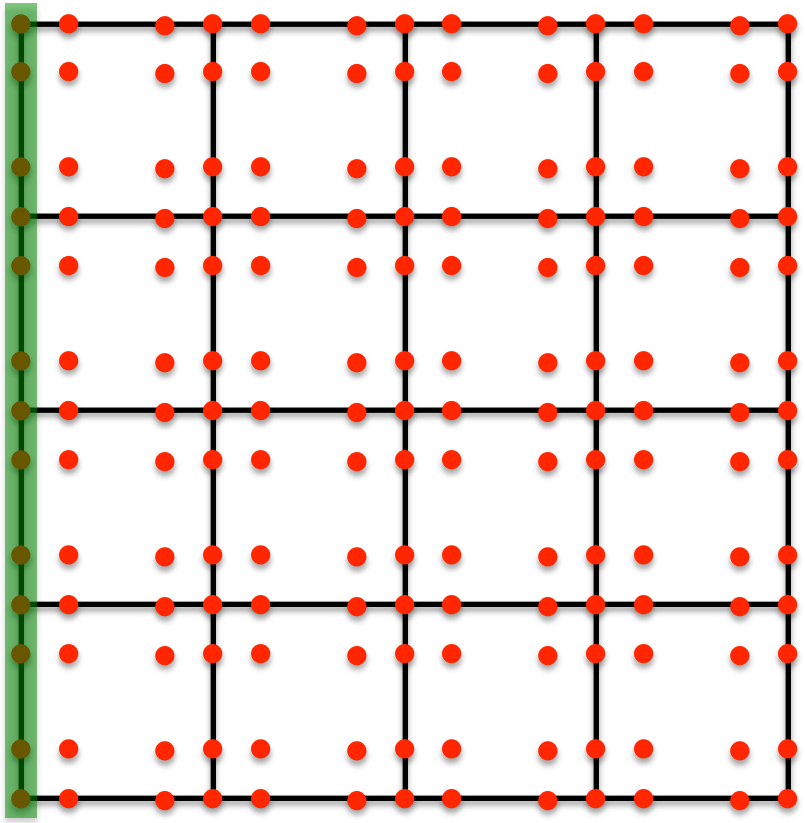

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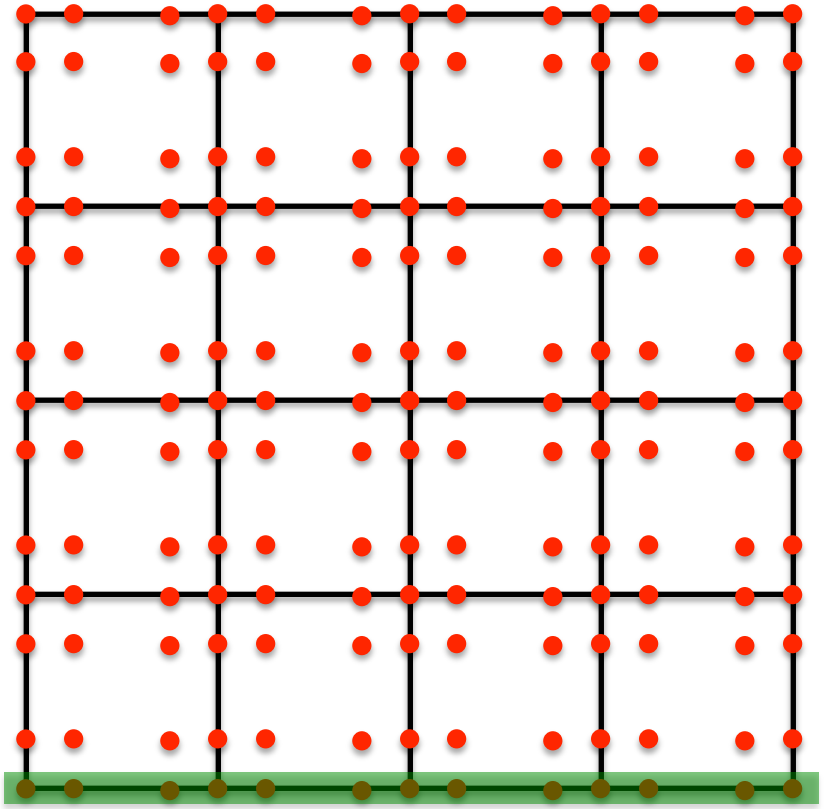

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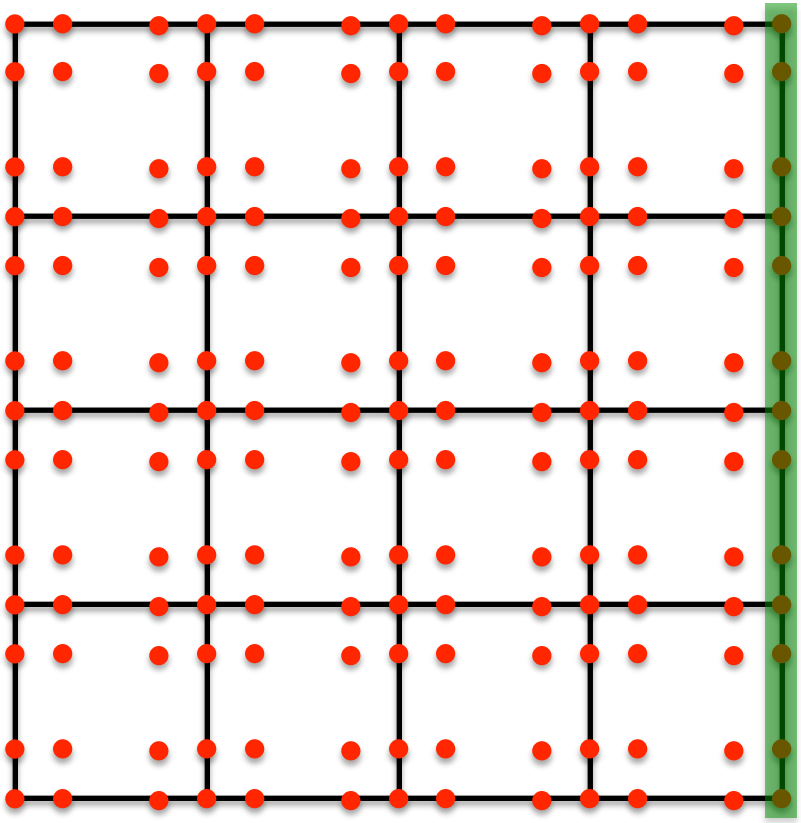

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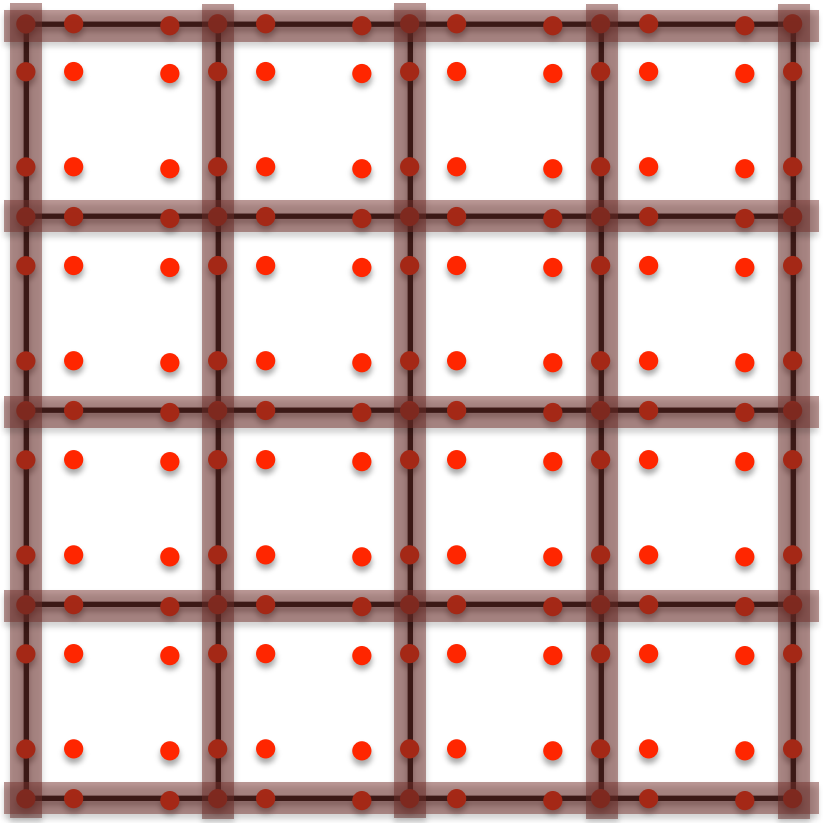
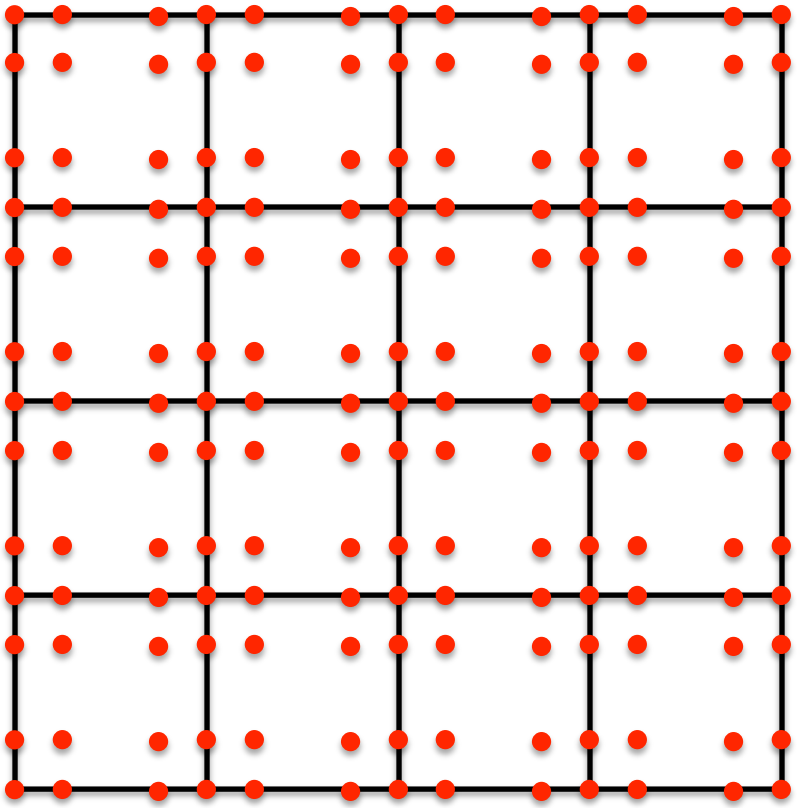


Optimizing Pack/Exchange/Unpack

- For a cycle, PCI-e D2H depends only on packing that cycle
  - Divide edge_pack into equal-sized cycles
    1. Find only the elements directly involved in each separate cycle
    2. Evenly divide remaining elements among the cycles
  - Associate each cycle with a unique CUDA stream
  - Launch each pack in its stream
  - After a cycle is packed, call async. PCI-e D2H in its Stream
- Edge_unpack at MPI boundaries requires all MPI to be finished
- However, internal unpacks can be done directly after packing

Porting Strategy: Pack/Exchange/Unpack

- For each cycle
  - Launch edge_pack kernel for the cycle in a unique stream
  - Call a cudaEventRecord for the stream's packing event



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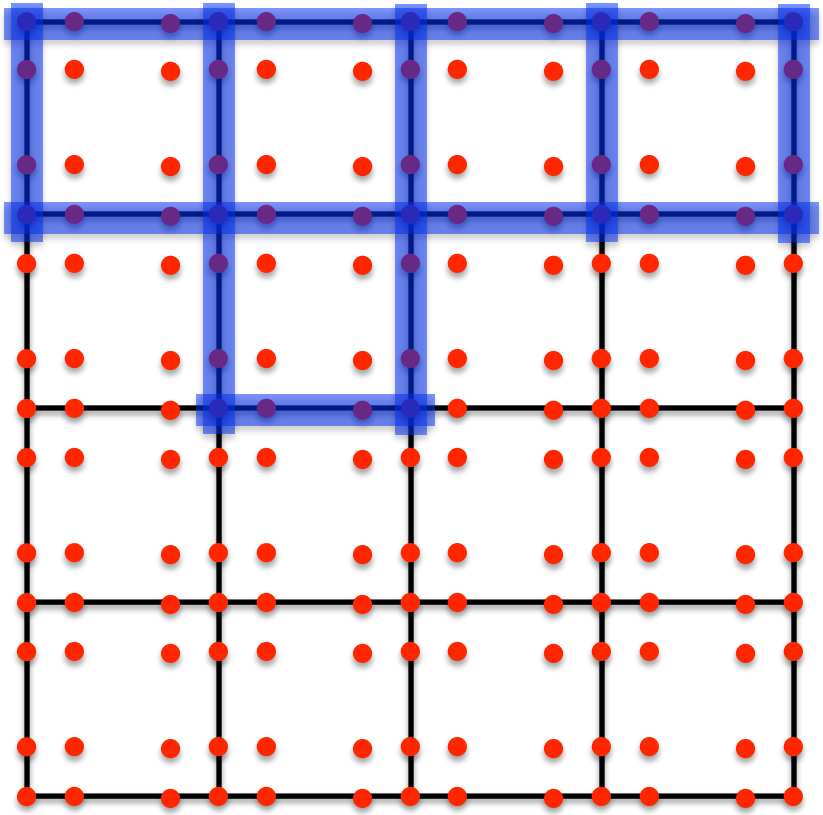

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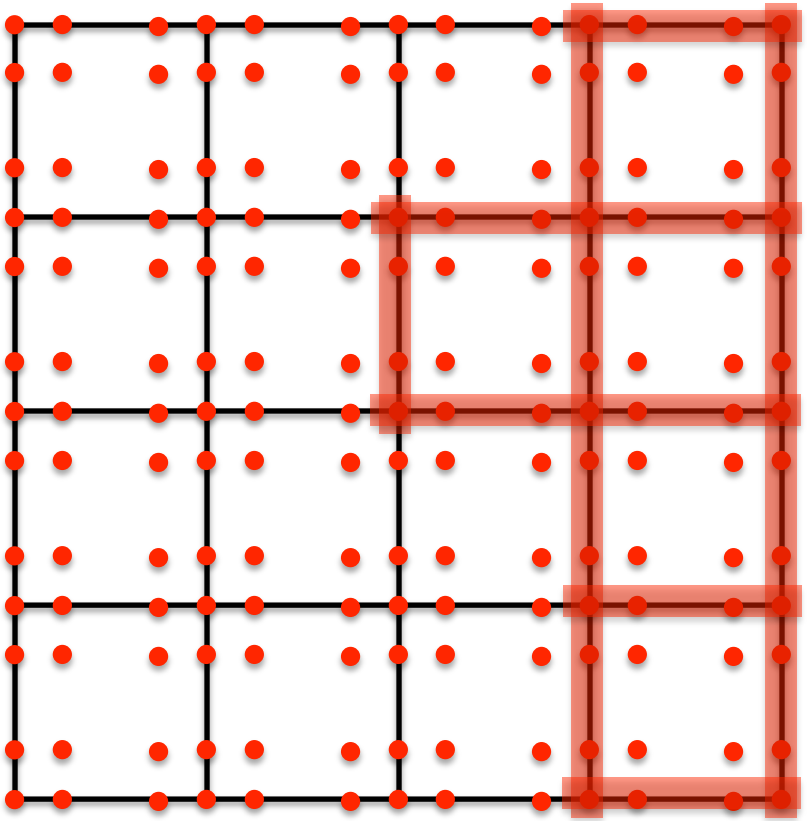

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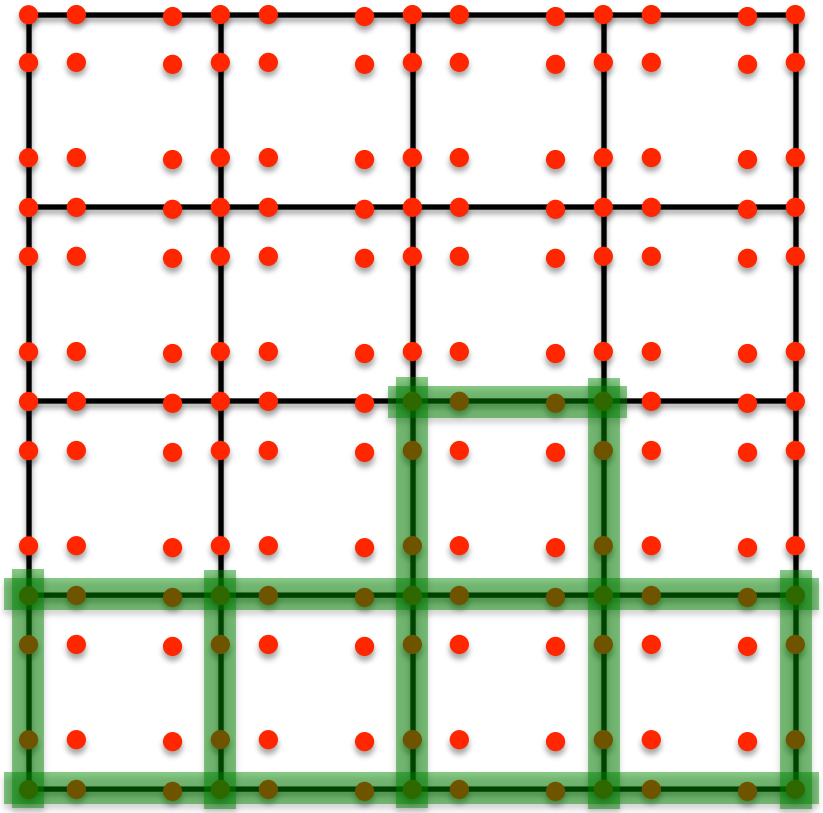

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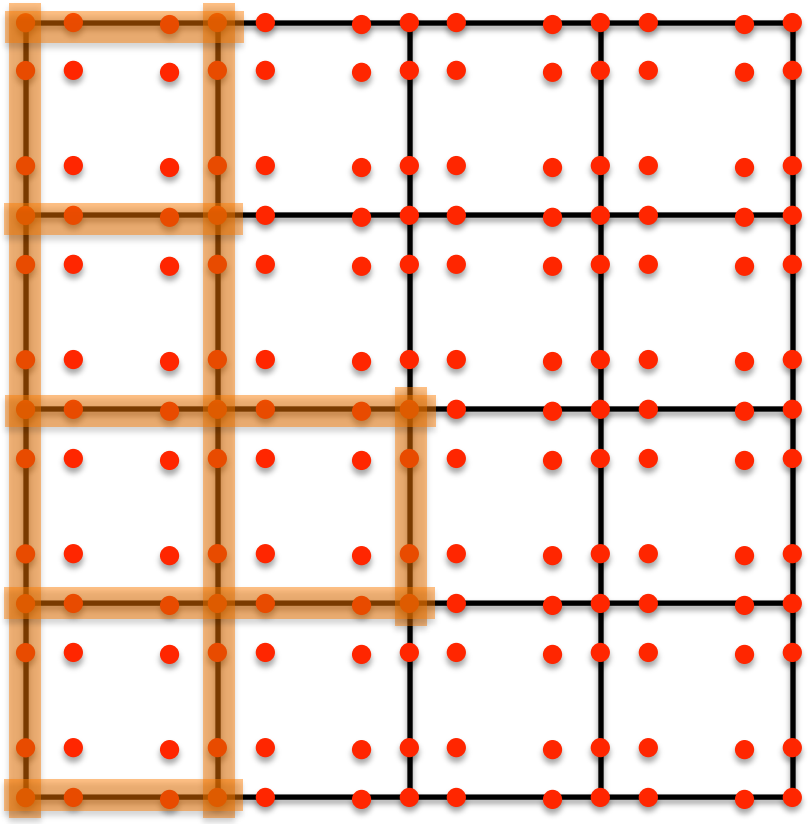

Other Important Porting Considerations

- Memory coalescing in kernels
  - Know how threads are accessing GPU DRAM

Think Differently About Threading

CPU Code

```
do ie=1,nelemd
 do q=1,qsize
  do k=1,nlev
   do j=1,np
    do i=1,np
     coefs(1,i,j,k,q,ie) = ...
     coefs(2,i,j,k,q,ie) = ...
     coefs(3,i,j,k,q,ie) = ...
```

GPU Code

```
ie = blockidx%y
q  = blockidx%x
k  = threadidx%z
j  = threadidx%y
i  = threadidx%x
coefs(1,i,j,k,q,ie) = ...
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However, this will not coalesce to fill the DRAM bus

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coefs(2,i,j,k,q,ie) = ...
coefs(3,i,j,k,q,ie) = ...
```

```
ie = blockidx%y
q  = blockidx%x
k  = threadidx%z
j  = threadidx%y
i  = threadidx%x
coefs(i,j,k,q,ie,1) = ...
coefs(i,j,k,q,ie,2) = ...
coefs(i,j,k,q,ie,3) = ...
```

Other Important Porting Considerations

- Memory coalescing in kernels
  - Know how threads are accessing GPU DRAM
- Use of shared memory
  - New vertical remap does nearly all computations on shared memory
  - Only accesses to DRAM are at start and end of a very large kernel
  - Hence, a 5.5x speed-up over CPU code for vertical remap
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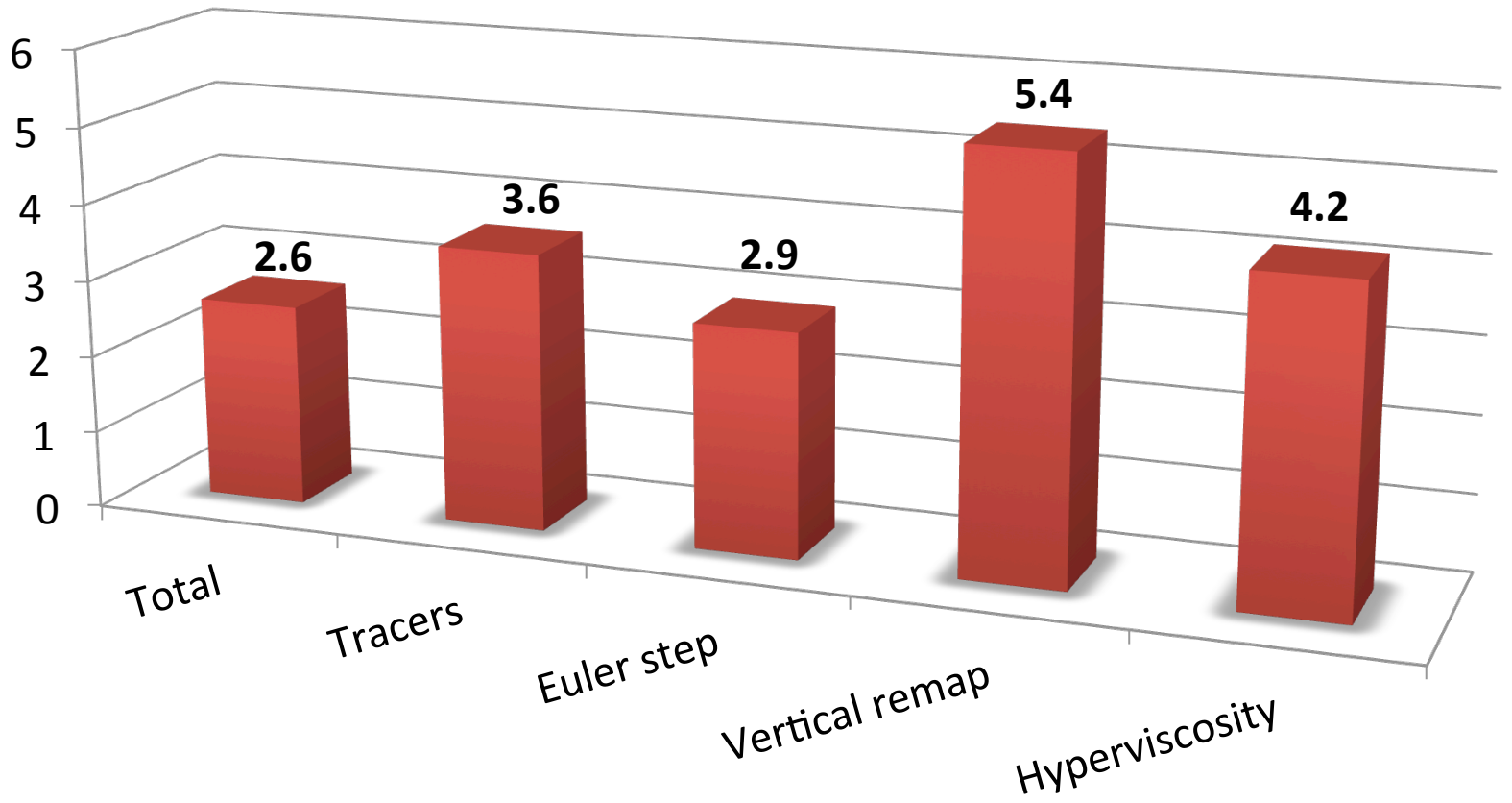
  - Computed & PCI-e copied data for future kernels during prior kernels
- PCI-e copies: consolidate if small, break up & pipeline if large

Speed-Up: Fermi GPU vs 1 Interlagos / Node

- Benchmarks performed on XK6 using end-to-end wall timers
- All PCI-e and MPI communication included



Computational Time-step barrier

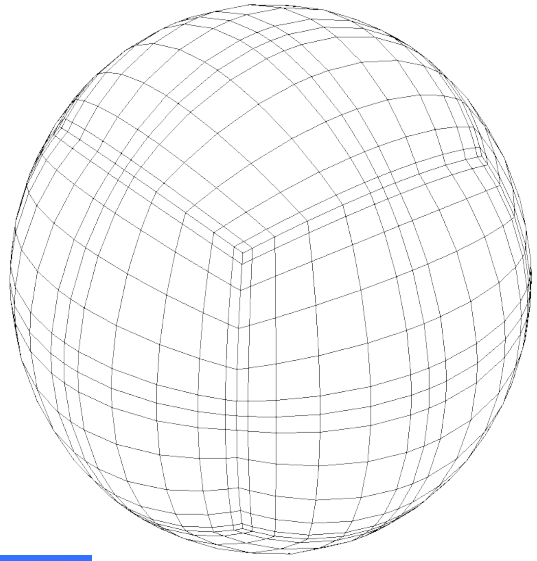
- Without it, climate simulation will hit the time-step barrier
  - Little benefit from higher scales of computing
  - Must choose between higher resolution or tolerable throughput
- Dramatically improve accuracy of highly-coupled models
- Dramatically accelerate spin-up of new simulations
- Potentially revolutionize climate simulation and other application areas with long time integration
- ***Crucial for climate simulation, promising for other fields***

Implicit versus Explicit

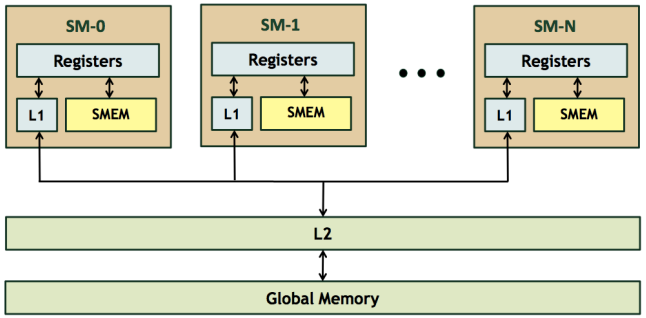
- *Explicit* time integration
  - Directly compute future state using derivatives at current or past times
  - Time step limited by numerical stability
- *Implicit* time integration
  - Define future state using derivates at that time, resulting in a system of (nonlinear) equations
  - Use (nonlinear) solver to determine future state
  - Numerically stable for large time steps
  - Time step limited by accuracy
  - Performance limited by solver

Accelerating Implicit solutions

Linking CAM-SE with third party software to create direct path to community algorithmic development

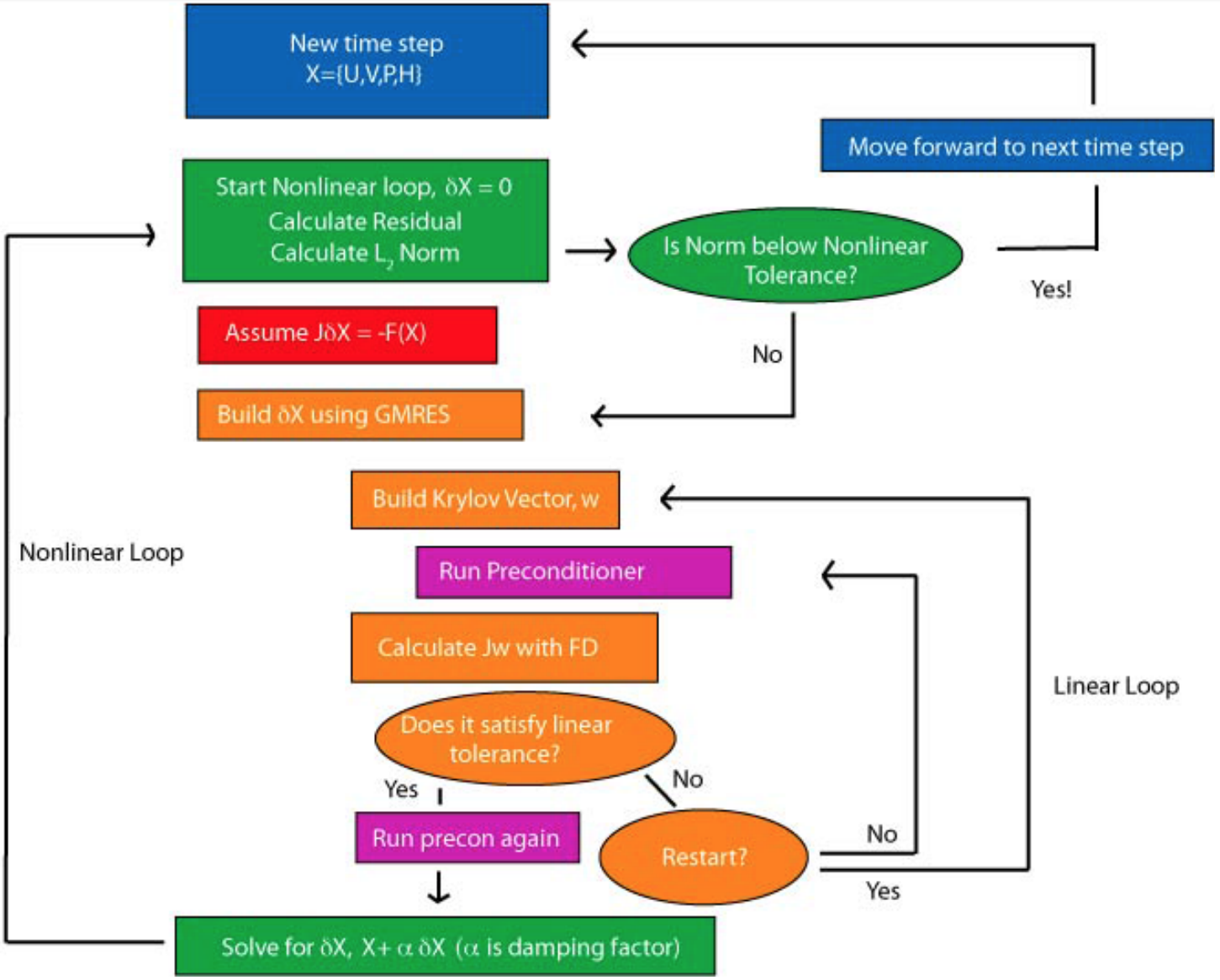


Linking CAM-SE with GPU community algorithmic development



Merging these separate efforts into the trunk of CAM-SE will allow accelerated time-stepping methods on hybrid architecture that keeps pass with community algorithmic development

Why Third Party Software?



JFNK Nested Algorithm

Modules available to CAM-SE

- **derived_type_mod**
  - type(derived_type) :: object (HOMME variables)
  - subroutine initialize(object, HOMME vars)
- **implicit_mod**
  - subroutine imp_solver(HOMME variables)
    - Set c_ptr -> f_ptr -> object
  - In c++, c_funptr points to calc_f in Fortran
  - subroutine calc_f(x(l), f(l), l, c_ptr) bind(C,name='user_sub_name')
- **noxlocainterface.cpp calls calc_f()**
- **noxlocainterface.hpp**

Next Steps – Implicit Framework

```
do n=1,nvar
 do ie=nets,nete
 do k=1,nlev
   do j=1,np
     do i=1,np
      lx = lx+1
      if (n==1) xstate(lx) = elem(ie)%state%v(i,j,1,k,np1)
      if (n==2) xstate(lx) = elem(ie)%state%v(i,j,2,k,np1)
      if (n==3) xstate(lx) = elem(ie)%state%p(i,j,k,np1)
     end do  !np
   end do  !np
 end do  !nlev
end do !ie
end do !nvar

call noxsolve(size(xstate), xstate, c_ptr_to_object, c_ptr_to_pre)

lx = 0
do n=1,nvar
 do ie=nets,nete
 do k=1,nlev
   do j=1,np
     do i=1,np
      lx = lx+1
      if (n==1) elem(ie)%state%v(i,j,1,k,np1)=xstate(lx)
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     end do  !np
   end do  !np
 end do  !nlev
end do !ie
end do !nvar

subroutine residual(xstate, fx, nelemd, c_ptr_to_object) bind(C,name='calc_f')

  use ,intrinsic :: iso_c_binding
  use kinds, only : real_kind
  use dimensions_mod, only : np, nlev, nvar, nelem
```

Next Steps – GPU Framework

```
subroutine remap_velocityQ_launcher(n0,np1,dt,elem,hvcoord,nets,nete,compute_diagnostics,rkstage)
  use hybrid_mod, only: hybrid_t

  ! Setup Thread Partitioning
  blockdim = dim3(np,np,_EUL_BLK_)
  griddim = dim3(qsize_d,int(ceiling(dble(nete-nets+1)/dble(_EUL_BLK_))),1)

  if(compute_mean_flux==1 .and. prescribed_wind==0) use_mean_flux=.true.

  do ie=nets,nete
    do i=1,np
      do j=1,np
        do k=1,nlev
            dp_np1_h(i,j,k,ie) = (hvcoord%hyai(k+1) - hvcoord%hyai(k))*hvcoord%ps0 + &
                                 (hvcoord%hybi(k+1) - hvcoord%hybi(k))*elem(ie)%state%ps_v(i,j,np1)

          endif
        enddo
      enddo
    enddo
  enddo
  ierr = cudaMemcpy(dp_star_d,dp_star_h,size(dp_star_h),cudaMemcpyHostToDevice)
  ierr = cudaMemcpy(dp_np1_d ,dp_np1_h ,size(dp_np1_h ),cudaMemcpyHostToDevice)

  ierr = cudaDeviceSetCacheConfig(cudaFuncCachePreferL1)
  call remap_velocityQ_kernel_new<<<griddim,blockdim>>>(n0,np1,dt,device_arrays%Qdp,nets,nete,comput
  ierr = cudaThreadSynchronize()

  call t_stopf('remap_velocityQ')

end subroutine remap_velocityQ_launcher
```

Next Steps – Linked Framework

```
      do n=1,nvar
       do ie=nets,nete
       do k=1,nlev
         do j=1,np
           do i=1,np
            lx = lx+1
            if (n==1) xstate(lx) = elem(ie)%state%v(i,j,1,k,np1)
            if (n==2) xstate(lx) = elem(ie)%state%v(i,j,2,k,np1)
            if (n==3) xstate(lx) = elem(ie)%state%p(i,j,k,np1)
           end do  !np
         end do  !np
       end do  !nlev
      end do !ie
      end do !nvar

   call noxsolve(size(xstate), xstate, c_ptr_to_object, c_ptr_to_pre)

      lx = 0
      do n=1,nvar
       do ie=nets,nete
       do k=1,nlev
         do j=1,np
           do i=1,np
            lx = lx+1
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           end do  !np
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       end do  !nlev
      end do !ie
      end do !nvar
  subroutine residual(xstate, fx, nelemd, c_ptr_to_object) bind(C,name='calc_f')

    use ,intrinsic :: iso_c_binding
    use kinds, only : real_kind
    use dimensions_mod, only : np, nlev, nvar, nelem
```

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  subroutine remap_velocityQ_launcher(n0,np1,dt,elem,hvcoord,nets,nete,compute_diagnostics,rkstage)
    use hybrid_mod, only: hybrid_t

    ! Setup Thread Partitioning
    blockdim = dim3(np,np,_EUL_BLK_)
    griddim = dim3(qsize_d,int(ceiling(dble(nete-nets+1)/dble(_EUL_BLK_))),1)

    if(compute_mean_flux==1 .and. prescribed_wind==0) use_mean_flux=.true.

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                                   (hvcoord%hybi(k+1) - hvcoord%hybi(k))*elem(ie)%state%ps_v(i,j,np1)

            endif
          enddo
        enddo
      enddo
    enddo
    ierr = cudaMemcpy(dp_star_d,dp_star_h,size(dp_star_h),cudaMemcpyHostToDevice)
    ierr = cudaMemcpy(dp_np1_d ,dp_np1_h ,size(dp_np1_h ),cudaMemcpyHostToDevice)

    ierr = cudaDeviceSetCacheConfig(cudaFuncCachePreferL1)
    call remap_velocityQ_kernel_new<<<griddim,blockdim>>>(n0,np1,dt,device_arrays%Qdp,nets,nete,comput
    ierr = cudaThreadSynchronize()

    call t_stopf('remap_velocityQ')

  end subroutine remap_velocityQ_launcher
```

Merge framework so that array state is manipulated once and ‘calc_f’ executes on the GPU

Future Efforts