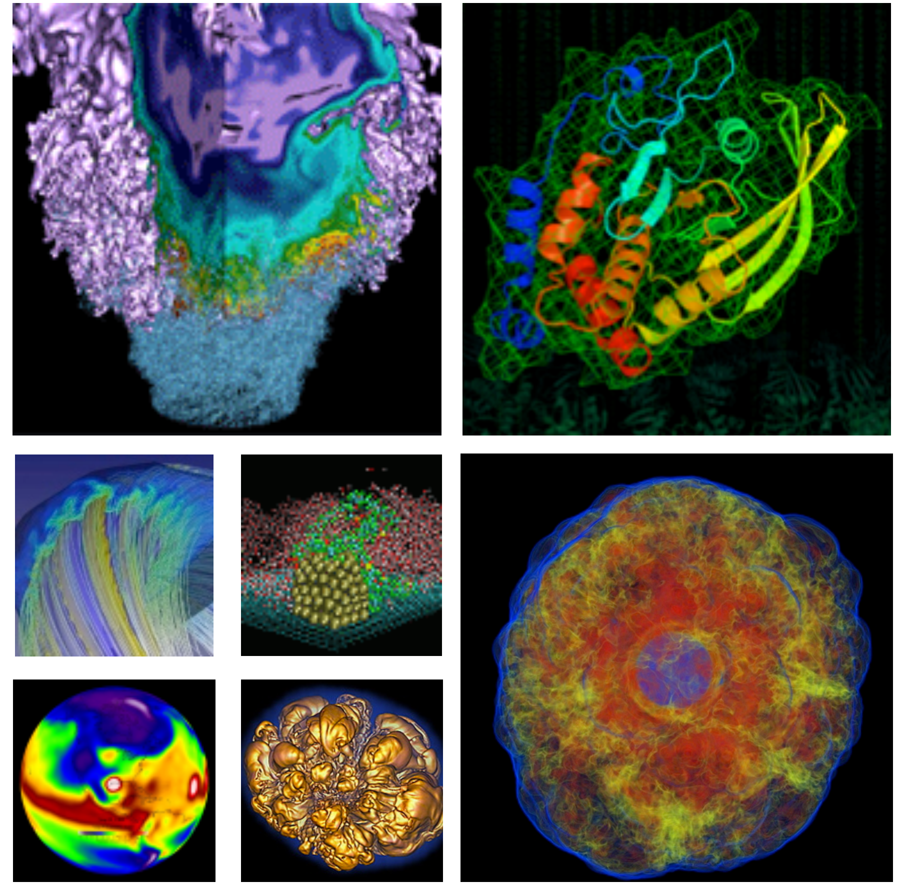
NESAP CESM MG2 Update



Helen He (and MG2 team)

Cray Quarterly Meeting
July 22, 2015

CESM NESAP MG2 Team Members

- **NCAR:** John Dennis, **Chris Kerr**, Sean Santos
- **Cray:** Marcus Wagner
- **Intel:** Nadezhda Plotnikova, Martyn Corden
- **NERSC Liaison:** Helen He

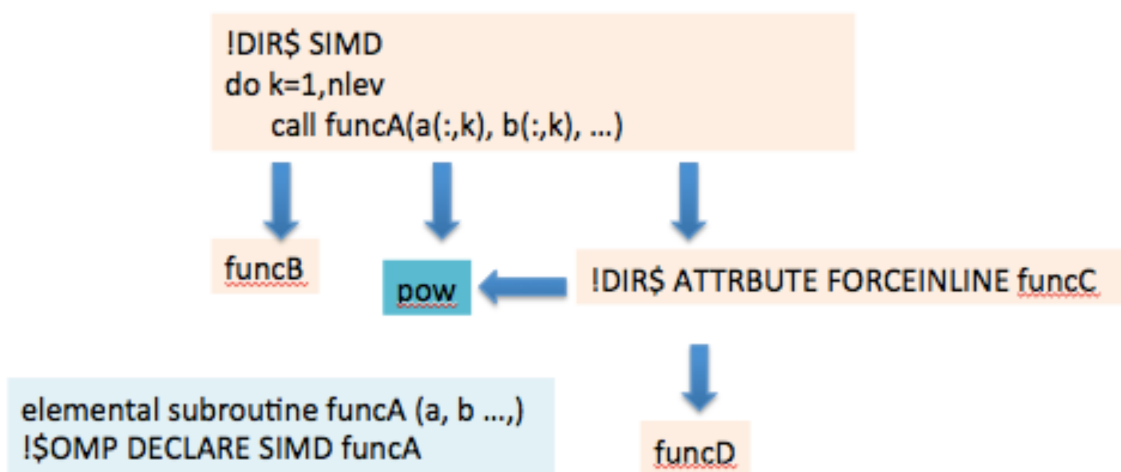
MG2 Kernel

- **MG2 is a kernel for CESM that represents its radiative transfer workload. Typically consumes about 10% of CESM run time.**
  - Brought to Dungeon Session in March
- **Kernel is core bound**
  - Not bandwidth limited at all
  - Shows very little vectorization
    - Some loop bounds are short (e.g. 10)
  - Heavy use of math instrinsics that do not vectorize
    - pow(), gamma(), log10().
    - Intel intrinsic gamma() is 2.6x slower than MG2 internal function
- **Kernel has long complex loops with interleaved conditionals and elemental function calls.**
  - Mixed conditionals and non-inlined functions inhibit vectorization
  - Some send array sections to elemental functions

MG2 Vectorization Prototype

- **Use compiler report to check and make sure key functions are vectorized (and all functions on the call stack are vectorized too)**
  - Elemental functions need to be inlined
  - “-qopt-report=5” reports highest level of details.
  - “-ipo” is needed if functions are in different source codes.
- **Add !$OMP DECLARE SIMD and !DIR$ ATTRIBUTE FORCEINLINE when needed.**

Example call stack for vectorization and inlining



Recommendations from Dungeon Session

- Divide major loops when possible and localize vectorization: work to be done by MG2 developers.
- Implement inlining as close to hotspot as possible; or use vector functions on the low level
- Follow up with MKL team on Gamma function vectorization.
- Work with compiler team for a flag to replace FORCEINLINE, and portable options for other compilers.

Changes Made to Improve Performance (1)

- **Remove 'elemental' attribute and move the 'mgncol' loop inside routine**

Before change:

```
elemental function
wv_sat_svp_to_qsat(es, p)
result(qs)

  real(r8), intent(in) :: es  !
SVP
  real(r8), intent(in) :: p
real(r8) :: qs

  ! If pressure is less than SVP,
set qs to maximum of 1.
  if ( (p - es) <= 0._r8 ) then
     qs = 1.0_r8
  else
     qs = epsilo*es / (p -
omeps*es)
  end if

end function wv_sat_svp_to_qsat
```

After change:

```
function wv_sat_svp_to_qsat(es, p,
mgncol) result(qs)
  integer,
intent(in) :: mgncol
  real(r8), dimension(mgncol),
intent(in) :: es  ! SVP
  real(r8), dimension(mgncol),
intent(in) :: p
  real(r8), dimension(mgncol) :: qs
  integer :: i
  do i=1,mgncol
  if ( (p(i) - es(i)) <= 0._r8 ) then
     qs(i) = 1.0_r8
  else
     qs(i) = epsilo*es(i) / (p(i) -
omeps*es(i))
  end if
  enddo
end function wv_sat_svp_to_qsat
```

Impact of Code Changes for Elemental Functions

- No changes to algorithm
- Algorithm gives same answers
- Code readability not effected
- Revised code looks almost identical to original
- Provide scalar and vector version of functions
- Overload function names to maintain single naming convention

Changes Made to Improve Performance (2)

- **Structure routine: don't use assumed-shaped arrays:**

```
Before change:
subroutine size_dist_param_liq(qcic, …,)
       real, intent(in) :: qcic(:)
   do i=1,SIZE(qcic)
```

```
After change:
subroutine size_dist_param_liq(qcic, …, mgncol)
       real, dimension(mgncol), intent(in) :: qcic
   do i=1,mgncol
```

Changes Made to Improve Performance (3)

- Divide loop blocks into manageable sizes. Allows compiler to vectorize loops. Can fuse loops during optimization step.
- Remove array syntax: plev(:,:) and replace with loops
- Replace divides: 1.0/plev(i,k) with *plev_inv(i,k)
- Remove initialization of variables that are over written

Changes Made to Improve Performance (4)

- **Rearrange loop order to allow for data alignment**

```
Before change:
do i=1,mgncol
      do k=1,nlev
        plev(i,k) = …
```

```
After change:
Do k=1,nlev
      do i=1,mgncol
        plev(i,k) = …
```

- **Use more aggressive compiler options**
  – -O3 -xAVX -fp-model fast=2 -no-prec-div -no-prec-sqrt -ip -fimf-precision=low -override-limits -qopt-report=5 -no-inline-max-total-size -inline-factor=200
- **Use Profile-guided Optimization (PGO) to improve code performance**
- **Compare performance of code with different vendors compilers**

Changes Made to Improve Performance (5)

- **Align data on specific byte boundaries; directive based approach with OMP directive:**
  - Portable solution:

    !$OMP SIMD ALIGNED (qc,qcn,nc,ncn,qi,qin,ni,nin,qr,qrn,nr,nrn,qs,qsn,ns,nsn)
    - Tells the compiler that the arrays are aligned
    - Asserts that there are no dependencies
    - Requires to use PRIVATE or REDUCTION clauses to ensure correctness
    - Forces the compiler to vectorize, whether or not it thinks if it is a good idea or not
  - As compared to:

    !DIR$ VECTOR ALIGNED
    - Tells the compiler that the arrays are aligned
    - Intel compiler specific, not portable
- **!$OMP SIMD ALIGNED is independent of vendor, however it can be overly intrusive in code**
- **8% improvement in overall performance**

!$OMP SIMD ALIGNED

- **The "ALIGNED" attribute is important for performance**
- **However, providing the list of variables for the aligned list is tedious and error-prone, and often times impossible in large real applications.**
  - !$OMP SIMD ALIGNED added in 48 loops in MG2 kernel, many with list of 10+ variables
- **Working with Intel compiler team to find a more manageable solution: How can compilers know better which arrays are aligned?**
- **Desired for other compilers too.**

!$OMP SIMD ALIGNED	!$OMP SIMD	!dir$ VECTOR ALIGNED	-align array64byte	-openmp	Time per iteration (usec) on Edison
x			x	x	444
x				x	446
	x		x	x	484
	x			x	482
		x	x		452
		x			456
					473

Srinath Vadlamani's testSIMD Suite

- Python test script to see which of the SIMD options are able to get close to AVX performance.
- "aligned" is essential
- Tests ran on Edison. Use "ifort" native compiler (15.0.1.133), default "-O2" optimization: not completely –no-vec

Compiler and language options	Run Time
None	4.0509
-xavx	3.2940
!$omp declare simd(init)	40.0168
!$omp declare simd(init) uniform(n)	40.0029
!$omp declare simd(init) simdlen(4) uniform(n)	37.8277
!$omp declare simd(init) simdlen(4)	37.7145
!$omp declare simd(init) **aligned(a:32)**	4.2609
!$omp declare simd(init) **aligned(a:32)** uniform(n)	4.2955
!$omp declare simd(init) simdlen(4**) aligned(a:32)**	4.2598
!$omp declare simd(init) simdlen(4) **aligned(a:32)** uniform(n)	4.2779

Performance Comparisons on Different Compilers and Hardware

Hardware	Compiler	Performance [usec per iteration]
Sandy-Bridge	Intel-15.0.2	541
Sandy-Bridge	PGI-15.5	600
Ivy-Bridge	Intel-15.0.1	407
Ivy-Bridge	Cray-8.3.11	347

- **Fastest run on Edison: 407 sec (not easily reproducible when run again with same executable)**
- **Original performance on Sandy-Bridge with Intel/15.0.2 is 1035 usec**
- **Cray compiler is fastest**

Summary

- Directives and flags can be helpful, however not a replacement for programmers work on code modifications.
- Break up loops and push loops into functions where vectorization can be dealt with directly and can expose logic to compiler.
- Incremental improvements not necessary a BIG win from any one thing. Accumulative results matter.
- Performance and portability is a major goal: use !$OMP SIMD proves to be beneficial but very hard to use regarding the need of providing the aligned list.

Thank you.