Optimizing NOAA/ESRL Weather Models for the Intel Xeon and Xeon Phi Architecture

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Jim Rosinski
NOAA/ESRL

Contributors

- Tom Henderson (NOAA)
  - Physics porting and optimization
- Jacques Middlecoff (NOAA)
  - MPI optimizations
- Mike Greenfield (Intel)
  - Organizing Intel assistance to FIM and NIM efforts
- Ruchira Sasanka (Intel)
  - Optimizing MPI communication
  - General optimization efforts
- Ashish Jha (Intel)
  - Alignment optimizations
  - Compiler flag suggestions

Outline

- Review
- Changes to NIM dynamics over the past year
- Current status of NIM dynamics performance
- Load balancing on heterogeneous hardware
- MPI bottlenecks
- Future directions

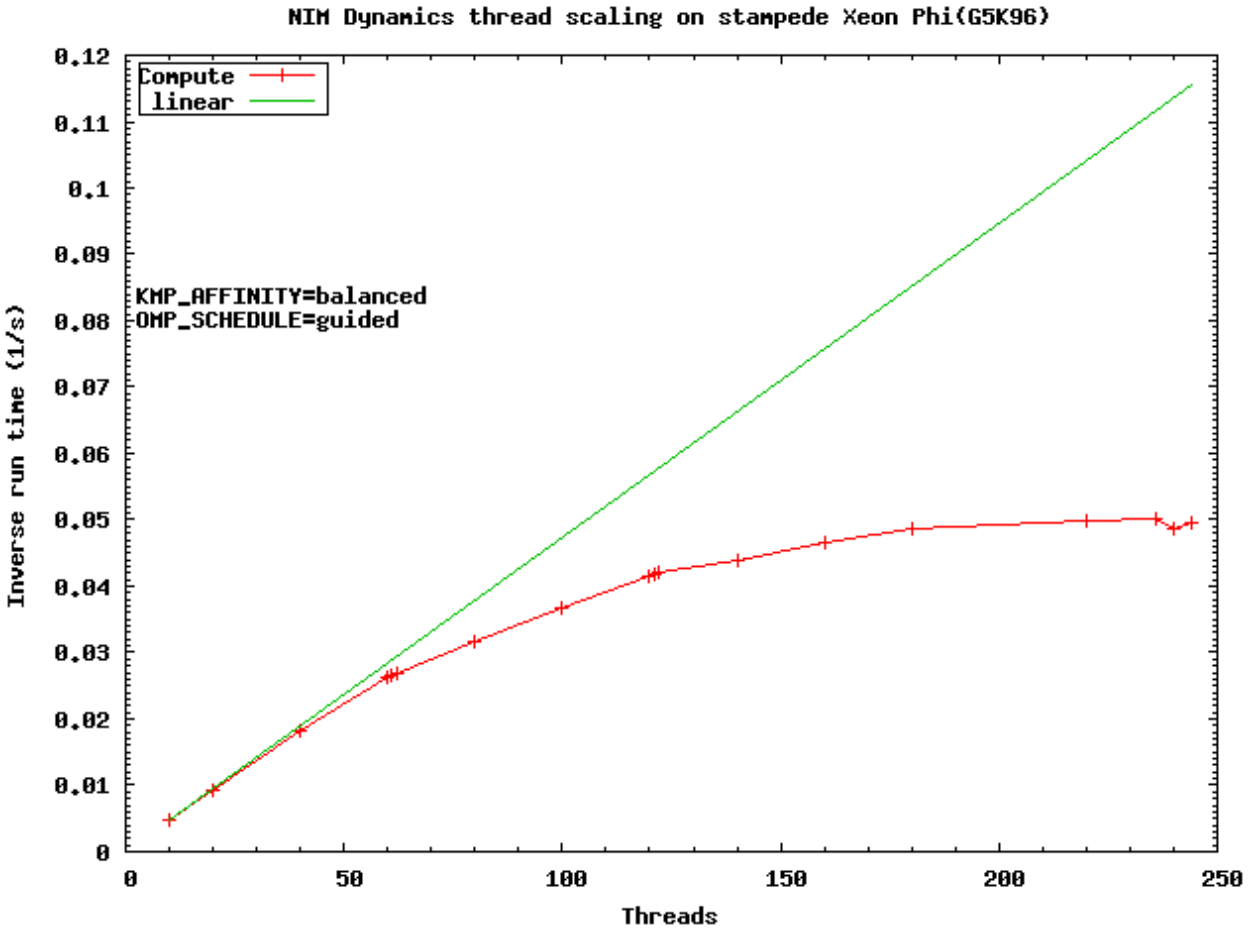
What is NIM?

- Non-hydrostatic Icosahedral Model
- Weather forecast model (up to 10 days)
  - Designed for very high resolution (< 10 km)
  - Improved forecast performance over terrain
- Software:
  - Optimize performance on current scientific target platform (Xeon-based)
  - Port to multiple platforms including fine-grained
  - Validate model solutions on all ported platforms

Review (last year at this time…)

- NIM dynamics successfully ported to KNC and GPU
- Symmetric mode works on SNB+KNC
- Good vectorization
- Good thread scaling

NIM thread scaling on KNC



Primary changes to NIM dynamics in 2014

- Truly single-source for CPU/KNC/GPU
  - Constraint: mods to 1 architecture cannot degrade performance on another
  - Very few architecture-specific ifdefs
- Ability to run in real*8 mode (Tom Henderson)
- Compute rather than read in giant arrays on initialization
  - Allows high resolution runs
- Special transcendental libraries allow bitwise-exact results host vs. KNC (thanks to Intel math libraries team)
- Changes to SMS library improve communication performance (Jacques Middlecoff)
  - Better threading helps CPU/KNC
  - Fewer kernel calls helps GPU
- Mods to diag.F90, trisol.F90 improve performance on CPU/GPU/KNC

NIM speedups on CPU due to hardware improvements

Architecture	CPU specs	Memory specs	NIM dynamics time on 1 node	% speedup vs. SNB
SandyBridge (stampede)	16 cores Intel Xeon E5-2680@2.7GHz	ddr3 1600 Mhz	92.1 sec	0%
IvyBridge (endeavor)	24 cores Intel Xeon E5-2697v2@2.7GHz	ddr3 1600 Mhz	67.1 sec	27%
Haswell-EP (endeavor)	28 cores Intel Xeon E5-2697v3@2.6Ghz	ddr4 2100 Mhz	57.4 sec	38%

Latest NIM G6K96 performance on various hardware (single-node)

Node configuration	MPI tasks	Runtime for 100 time steps	Hardware specs (system=Intel endeavor)
Host-only IVB	2	67.1 sec	Xeon E5-2697v2, 2.7 GHz, 24 cores
Host-only HSW-EP	2	57.4 sec	Xeon E5-2697v3, 2.6 GHz, 28 cores
KNC-only	2	67.4 sec	1.23 GHz, 61 cores
Symmetric IVB+KNC	5+5	39.6 sec	See above

Two simple but important mods affecting host and KNC performance

Runtime PRIOR to code mods (sec)		
Routine	SNB	KNC
diag	6.2	1.5
trisol	0.5	1.5

Runtime AFTER code mods (sec)		
Routine	SNB	KNC
diag	4.7	1.4
trisol	0.5	0.4

Host compiler issue (diag.F90)

- Vector loop gets fused with scalar loop:

```
! Line 93: This loop cannot vectorize due to a dependency
 do k=nz-1,0,-1
   p(k,ipn) = p(k+1,ipn) + pdel(k+1)
 end do

! Line 111: This loop can easily vectorize
 do k=1,nz
   term(k) = rd*tr(k,ipn)*1.e-5_rt
 end do

diag.f90(93): (col. 5) remark: loop was not vectorized: existence of vector dependence
Fused Loops: ( 93 111 )
```

- Solution: add “nofusion” directives to unvectorizable loops:

```
! Line 93: This loop cannot vectorize due to a dependency
!DIR$ NOFUSION
 do k=nz-1,0,-1
   p(k,ipn) = p(k+1,ipn) + pdel(k+1)
 end do
```

KNC compiler issue (trisol.F90)

- Vector loop gets fused with scalar loop:

```
! Line 97: This loop can vectorize even though it has many computations
  do k=1,nz-1
    kp1 = k+1
    km1 = k-1
    thkp1 = .5_rt*( bedgvar(kp1,ipn,6)+bedgvar(k,ipn,6))
    thkp  = .5_rt*( bedgvar(km1,ipn,6)+bedgvar(k,ipn,6))
... Lots more vectorizable code
  end do
...
! Line 139: This loop cannot vectorize because there is a dependency (w1d)
 do k=2,nz
    alpha = 1._rt/(bbb(k)-aaa(k)*gama(k-1))
    gama(k) = ccc(k)*alpha
    w1d(k) = (rrr(k)-aaa(k)*w1d(k-1))*alpha
 end do
```

- ifort -opt-report-phase=hlo -vec-report6 says:

```
fused Loops: ( 97 139 )
fused Loops: ( 84 97 )
trisol.f90(84): (col. 3) remark: loop was not vectorized: existence of vector dependence
```

KNC compiler issue (trisol.F90 cont'd)

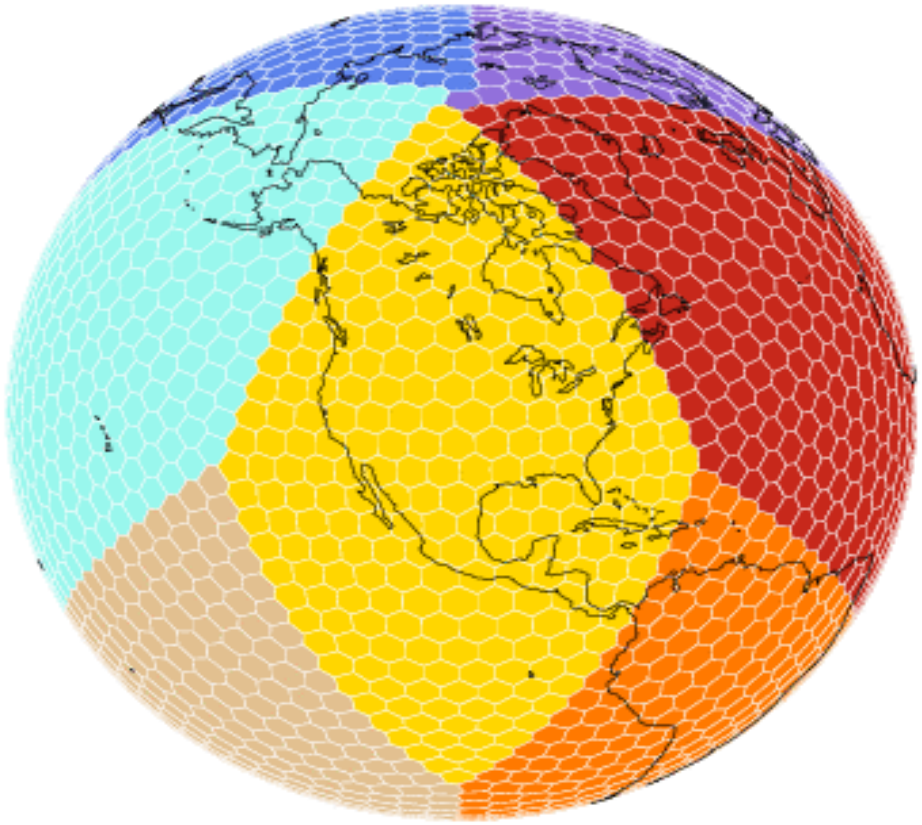
- Solution: add "nofusion" directive to unvectorizable loop:

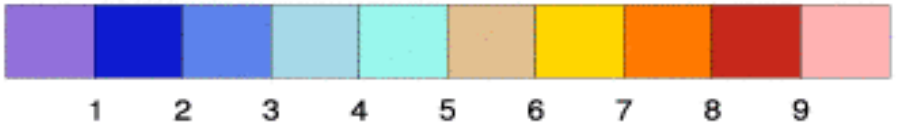
```
! Line 139: Disallow loop fusion of unvectorizable loop
!DIR$ NOFUSION
 do k=2,nz
    alpha = 1._rt/(bbb(k)-aaa(k)*gama(k-1))
    gama(k) = ccc(k)*alpha
    w1d(k) = (rrr(k)-aaa(k)*w1d(k-1))*alpha
 end do

trisol.f90(84): (col. 3) remark: FUSED LOOP WAS VECTORIZED
```

Validation

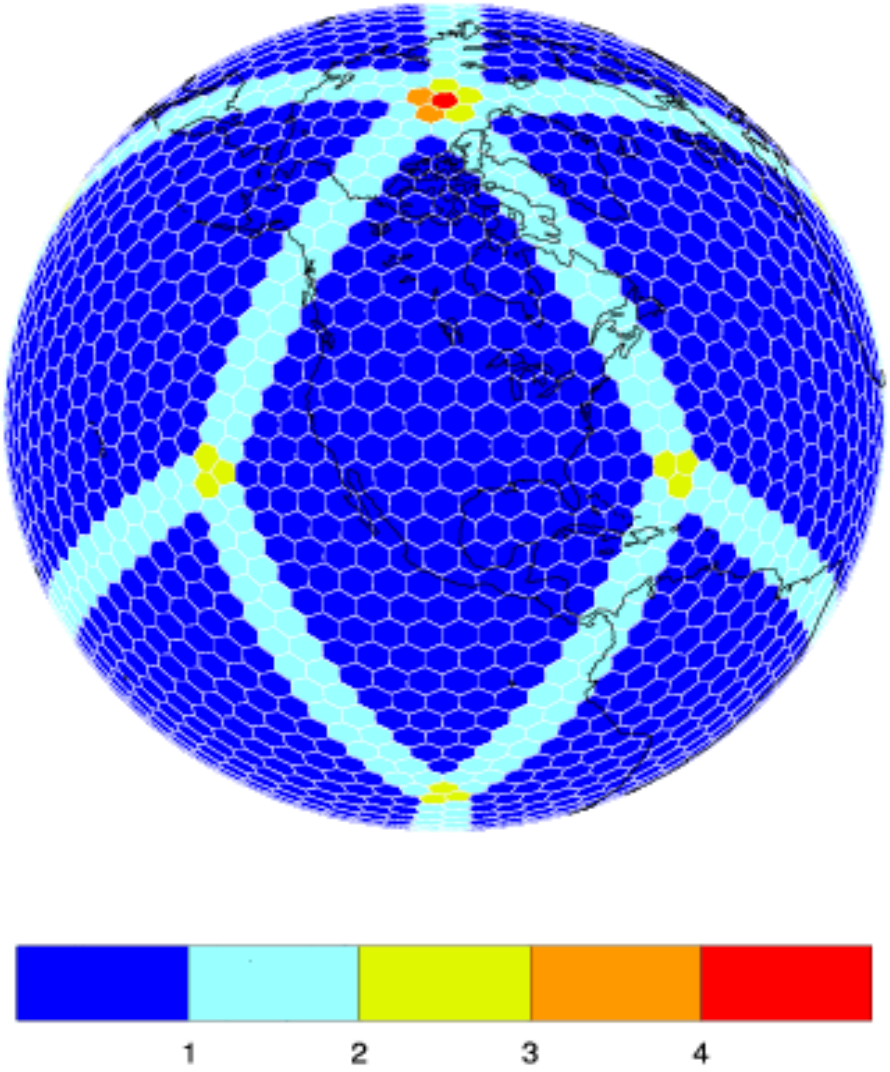
- NIM dynamics can be made to produce bitwise-identical answers Xeon vs. Phi if canonical transcendental functions are used.
  - No reductions which feed back into model calculations (vector, OMP, or MPI)
- Software constraint: NIM must produce bitwise identical answers across varying MPI task counts
  - -fp-model precise required on host compilation
- Intel provided us prototype math libraries for Xeon and Phi that produce bitwise identical results for transcendental functions (e.g. exp, log, pow, sin, cos). The library is not performance optimized, but allows us to unambiguously validate the port to Phi.

NIM G4 point allocation on 10 MPI tasks





NIM G4 10 MPI: Number of sends for each grid point



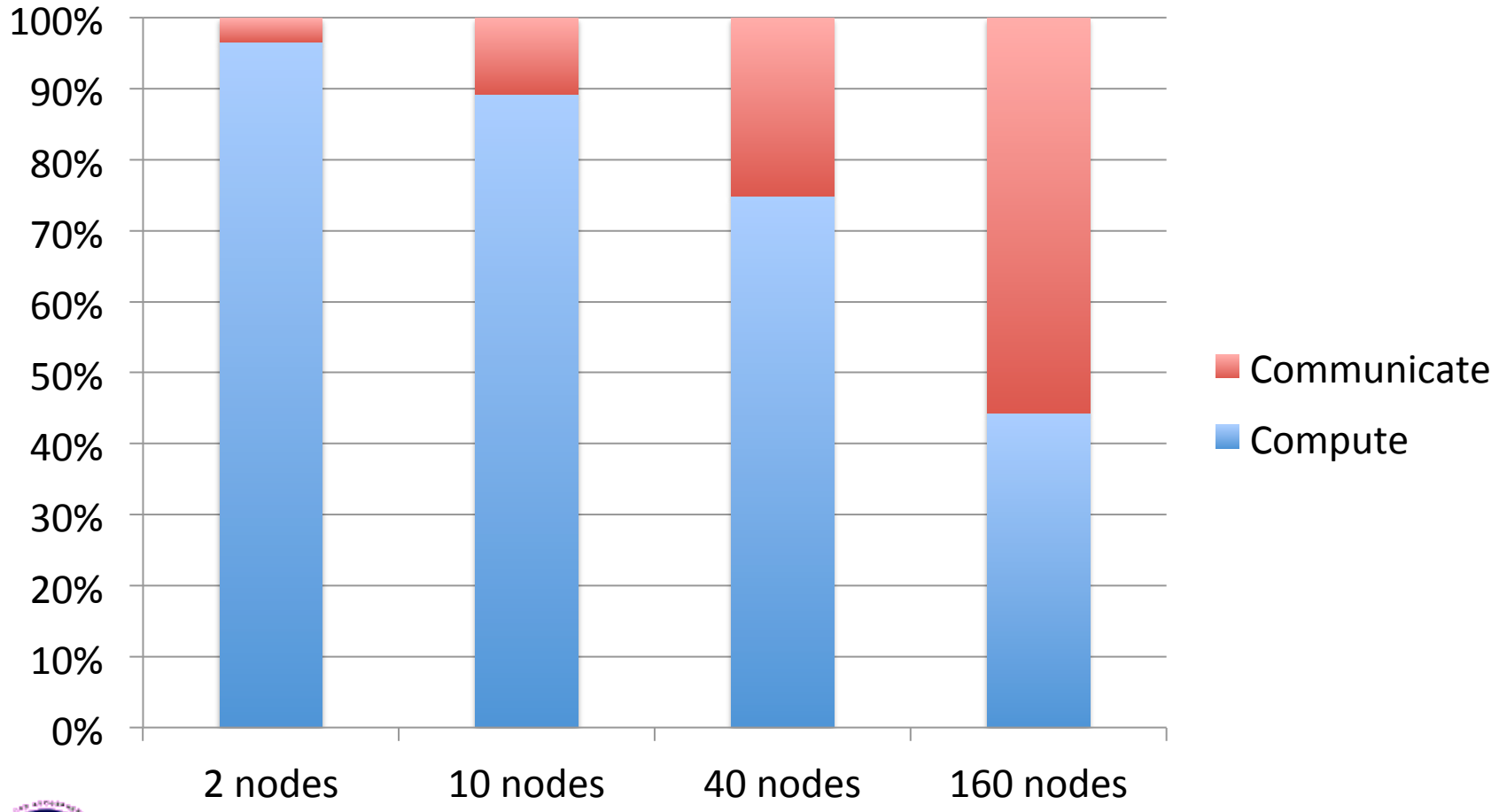
Symmetric mode load balancing

name	ncalls	nranks	mean_time	std_dev	wallmax	(rank)	wallmin	(rank)
Diag	1002	2	3.314	1.979	4.713	(0)	1.914	(1)
MainLoop	2	2	50.294	0.176	50.419	(0)	50.170	(1)
ZeroTendencies	200	2	0.093	0.022	0.108	(0)	0.077	(1)
SaveFlux	200	2	0.149	0.052	0.186	(0)	0.112	(1)
Dyntnc	800	2	38.277	1.794	39.546	(1)	37.009	(0)
RHStendencies	800	2	0.419	0.139	0.518	(0)	0.321	(1)
Vdm	800	2	23.368	2.984	25.478	(0)	21.258	(1)
Vdmintv	800	2	6.462	0.282	6.661	(0)	6.262	(1)
Vdmints0	800	2	5.567	0.693	6.057	(0)	5.076	(1)
Vdmints3	800	2	8.506	1.037	9.240	(0)	7.773	(1)
vdmfinish	800	2	2.820	0.986	3.517	(0)	2.122	(1)
Vdn	800	2	1.806	0.224	1.965	(0)	1.648	(1)
Flux	800	2	3.676	0.105	3.750	(0)	3.601	(1)
Force	800	2	1.650	0.071	1.700	(0)	1.600	(1)
RKdiff	800	2	1.411	0.197	1.551	(0)	1.271	(1)
TimeDiff	800	2	0.706	0.237	0.873	(0)	0.538	(1)
Sponge	800	2	0.365	0.088	0.427	(0)	0.303	(1)
pre_trisol	200	2	0.139	0.019	0.153	(1)	0.126	(0)
Trisol	200	2	0.416	0.114	0.497	(0)	0.336	(1)
post_trisol	200	2	0.076	0.004	0.079	(0)	0.073	(1)
Vdmints	200	2	3.499	0.303	3.714	(0)	3.285	(1)
Pstadv	200	2	0.792	0.029	0.813	(1)	0.772	(0)

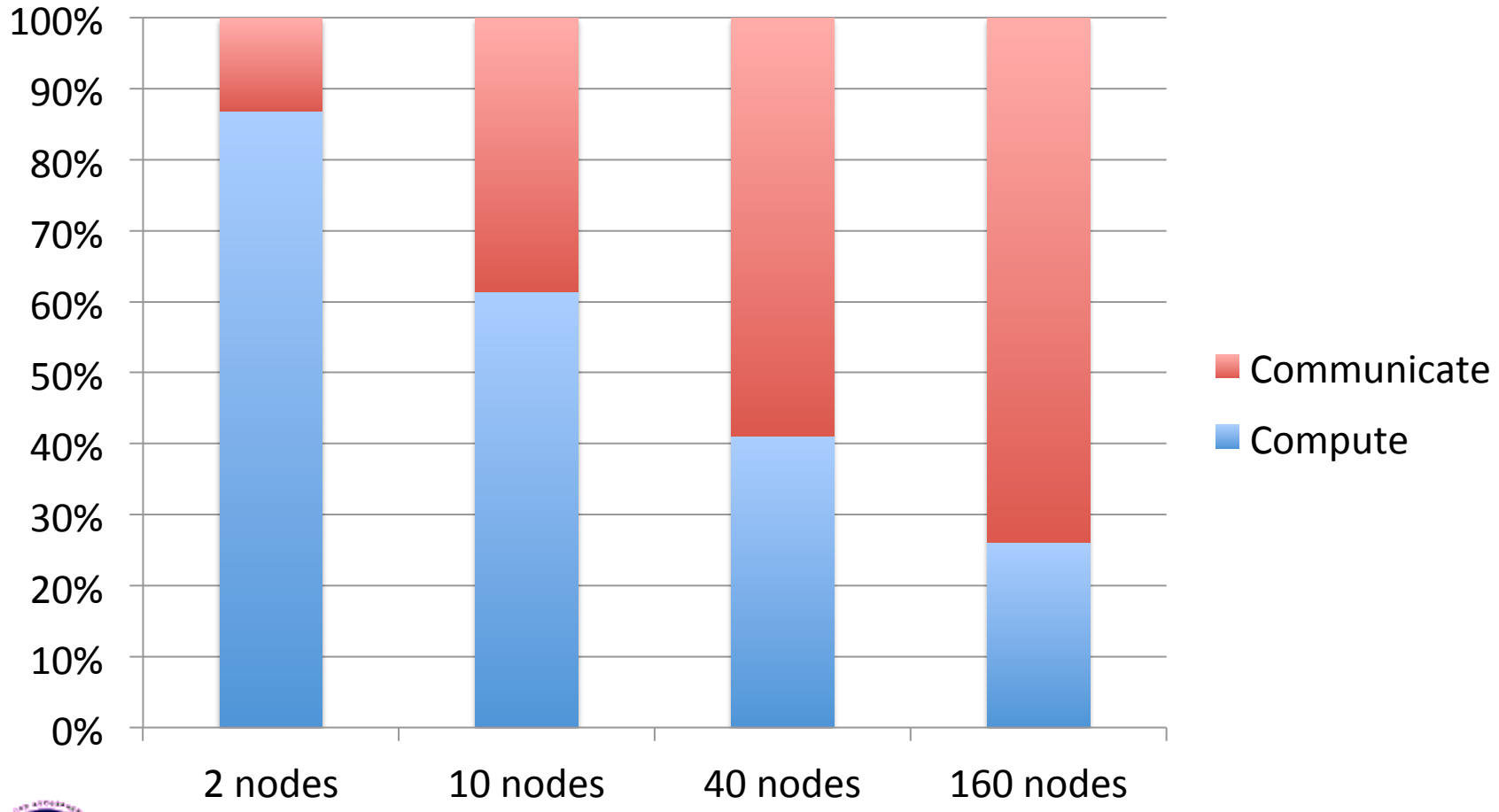
Symmetric mode load balancing (cont'd)

name	ncalls	nranks	mean_time	std_dev	wallmax	(rank)	wallmin	(rank)
Diag	5010	10	2.494	1.070	3.766	(0)	1.616	(9)
MainLoop	10	10	47.567	0.111	47.697	(2)	47.480	(8)
ZeroTendencies	1000	10	0.071	0.009	0.094	(0)	0.063	(1)
SaveFlux	1000	10	0.103	0.022	0.135	(2)	0.078	(4)
Dyntnc	4000	10	37.124	0.889	37.863	(7)	36.022	(0)
RHStendencies	4000	10	0.316	0.042	0.357	(1)	0.243	(9)
Vdm	4000	10	22.724	2.322	24.622	(9)	19.964	(3)
Vdmintv	4000	10	6.513	1.062	7.361	(8)	5.253	(3)
Vdmints0	4000	10	5.506	0.637	6.026	(9)	4.749	(3)
Vdmints3	4000	10	8.442	1.002	9.389	(9)	7.264	(1)
vdmfinish	4000	10	2.243	0.394	2.726	(0)	1.815	(9)
Vdn	4000	10	1.623	0.101	1.710	(8)	1.451	(3)
Flux	4000	10	3.629	0.509	4.053	(4)	3.020	(0)
Force	4000	10	1.487	0.147	1.639	(9)	1.299	(2)
RKdiff	4000	10	1.074	0.108	1.202	(1)	0.913	(6)
TimeDiff	4000	10	0.583	0.060	0.665	(0)	0.520	(6)
Sponge	4000	10	0.284	0.007	0.299	(0)	0.274	(1)
pre_trisol	1000	10	0.076	0.009	0.088	(0)	0.064	(9)
Trisol	1000	10	0.392	0.006	0.400	(2)	0.385	(9)
post_trisol	1000	10	0.057	0.009	0.065	(7)	0.045	(3)
Vdmints	1000	10	3.493	0.482	3.900	(9)	2.918	(3)
Pstadv	1000	10	0.803	0.162	0.944	(4)	0.611	(1)

G6K96 relative cost compute vs. communicate on SNB



G6K96 relative cost compute vs. communicate on KNC



Breakdown of MPI cost on SNB: 10 nodes

EXCHANGE OPERATON	MINIMUM	MEAN	MAXIMUM
Pack(seconds)	1.5155	1.5712	1.7117
MPI_Isend(seconds)	0.1763	0.2225	0.3185
MPI_Irecv(seconds)	0.0415	0.0495	0.0614
MPI_Waitall(seconds)	7.0462	7.4773	7.7944
Unpack(seconds)	1.1498	1.3451	1.5859

Breakdown of MPI cost on KNC: 10 nodes

EXCHANGE OPERATON	MINIMUM	MEAN	MAXIMUM
Pack(seconds)	8.1820	9.1503	11.8154
MPI_Isend(seconds)	1.6955	2.1908	2.7045
MPI_Irecv(seconds)	0.3458	0.4212	0.5344
MPI_Waitall(seconds)	27.7297	28.9001	30.1728
Unpack(seconds)	8.2697	9.3052	12.0066

Where Next?

- Further enhance communication
  - Why is pack/unpack performance so much worse on KNC?
  - Try replacing MPI_Isend with MPI_Irsend since message sizes are large?
  - Improvements to KNC performance should also help host
- FIM in symmetric mode

Summary

- Full NIM dynamical core ported to Xeon Phi using symmetric mode
  - Scientists are working on topography
- Single-source for CPU, Phi, GPU
- Dynamics running reasonably well on Phi (performance matches IVB node)
- Biggest performance bottleneck is MPI

Backup slides

Multi-core performance (32-bit)

- Peak on SNB: 16 cores * 8 flops/clock/core * 2 vector instructions * 2.6 GHz = 665.6 Gflops/s
- NIM observed on SNB: 1.63e12 flops / 22.423 sec / 665.6e9 peak flops= 11% of peak

- Peak on KNC: 61 cores * 16 flops/clock/core * 1.238 GHz = 2.416 Tflops/s
- NIM observed on KNC: 1.63e12 flops / 22.254 sec / 2.416e12 peak flops/s = 3% of peak

- NIM observed on K20X GPU: 1.63e12 flops / 17.924 sec / 3.95e12 peak flops/s = 2% of peak

Pack/Unpack code

```
do varNumber = 1,IVRBL
  var => exchPtr(varNumber)%varptr
  do n = 1,NumSendsOrRecvs
!$OMP PARALLEL DO PRIVATE (jindirect, offset, i)
    do j = 1,numberToPackOrUnpk(n,varNumber)
      jindirect = varIndexes(j,n,varNumber)
      offset    = bufIndexes(j,n,varNumber)
      if(pack) then !Pack the buffer
        do i = js(varNumber),je(varNumber)
          buffer(i+offset,n) = var(i,jindirect)
        enddo !i
      else ! Unpack the buffer
        do i = js(varNumber),je(varNumber)
          var(i,jindirect) = buffer(i+offset,n)
        enddo !i
      endif !pack
    enddo !j
  enddo !n
enddo !varNumber
```