



HPC Asia 2019 Guangzhou, Jan 14, 2019

Strategy of the code modernization optimization for ocean numerical model: A case study of MASNUM wave model Zhenya Song^{*, +}

Xiaodan Yang *,+

* First Institute of Oceanography (FIO), State Oceanic Administrative (SOA), China + Intel[®] Parallel Computing Center at FIO

Outline

- Brief Introduction of Intel[®] PCC at FIO
- Background
- Optimization strategy
- Future work

- MNR Headquarters, Beijing
- * 4 Research Institute
- FIO, Qingdao
- SIO, Hangzhou
- TIO, Xiamen
- 4IO, Beihai (being built)
- 8 Operational Centers
- NMEFC, NMEMC, NMDIS...
- 3 Branches
- North Sea, East Sea, South Sea



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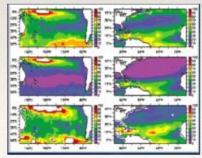
Mission

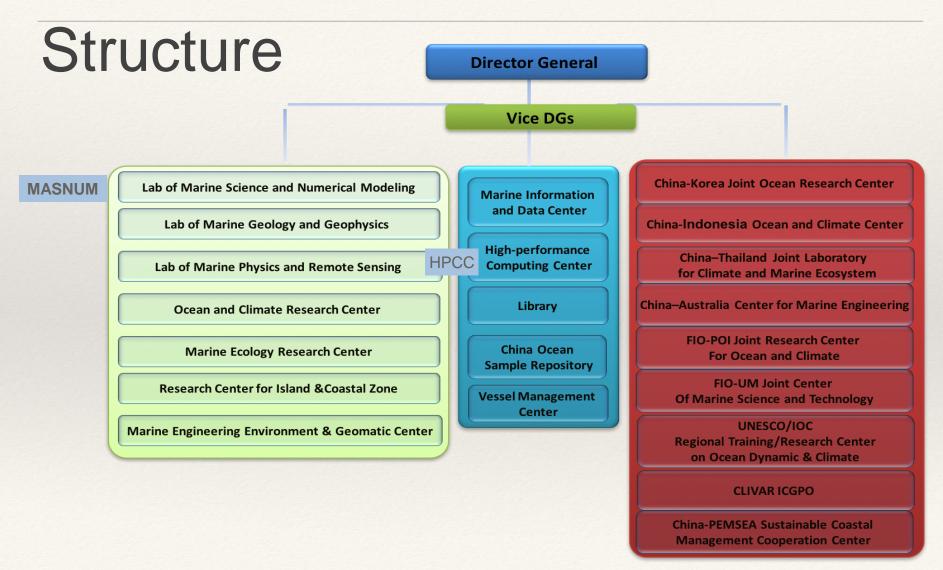
- Basic and applied research in oceanography, marine science and technology.
- Technical support and research service to the development of hightech industries, marine resources management, marine environment protection, public service, marine safety, etc.
- Major research priorities: Marine Geology/Geophysics, Physical Oceanography, Sea-Air Interaction, Marine Ecology, Marine Engineering, Remote Sensing, Marine Policy, etc.











MASNUM Major Research Fields

- Oceanography dynamics in the Chinese offshore area, polar region and global oceans
- Formation and variation mechanisms of major marine phenomena and circulation systems in the Chinese offshore area, polar region and global oceans
- General ocean circulation, mass transport and its ecological effect
- Land-sea-air interaction and climate changes
- Ocean survey and experiment techniques
- Sound, light and electricity measurement techniques
- Wave tank and physical model experiments
- Survey technique application and data process in oceanography
- Ocean numerical modeling
- Numerical computing scheme and data analysis
- Wind-wave-current interaction mechanism and coupled numerical model
- Application systems including database and data assimilation technique
- Marine information system
- Database, visualization and system integration techniques
- Application information systems in climate forecast, disaster prediction, engineering oceanography and military security

Intel[®] PCC at FIO

Large-Scale and Highly-Effective Numerical Simulation of Marine Environment with Global Surface Waves Model



Fangli Qiao



Xiaomeng Huang



Zhe Wang



Yanguo Yang



Shan Zhou



Haifeng Lv

 Optimize the MASNUM wave model

- Computing performance— Better Scalability and simulation faster
- Simulation ability—More accuracy by using deep learning
- Release the code to the ocean community worldwide
- Publish papers in SCI/EI journal
- Training course, and workshop of best known method sharing

Intel[®] PCC at FIO

Large-Scale and Highly-Effective Numerical Simulation of Marine Environment with Global Surface Waves Model



- Project period
- July 1, 2018—June 30, 2020
- Unveiling ceremony on July 28, 2018, Qingdao
- First one in Chinese ocean fields

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Ocean surface wave

- Occur in the ocean surface driven by winds
- Wave height range from several centimeters to tens meters

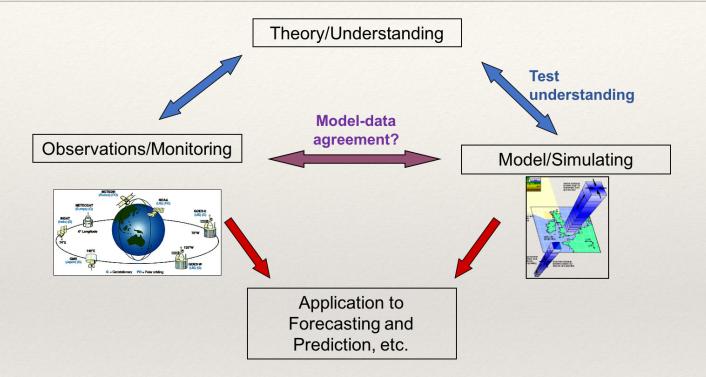


Importance of ocean surface wave



Ocean surface wave is important for navigation.

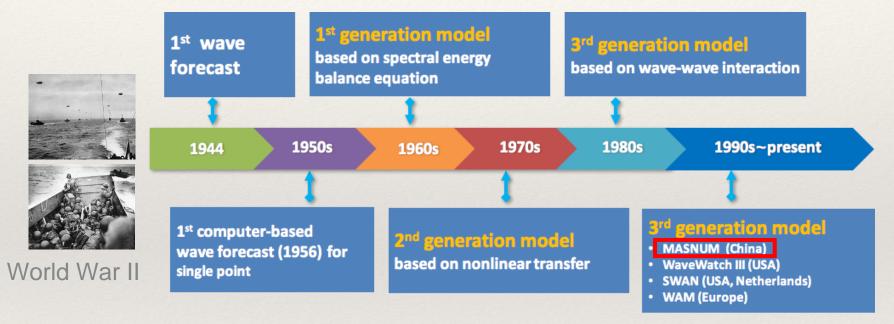
* Ocean surface wave is important for ocean engineering



 Three methods: Theoretical research, Lab experiments and Observation, and Numerical simulation

Model is the key tool for forecasting and prediction

History of ocean surface wave model



* First ocean surface wave forecasting during World War II (1944)

- * Ocean surface wave model is the key tool to wave forecasting
- * Accurately ocean surface wave forecasting is still a challenge

Model equation

Equation

$$\frac{\partial E}{\partial t} + \left(\frac{C_{g\lambda} + U_{\lambda}}{R\cos\phi}\right) \frac{\partial E}{\partial \lambda} + \left(\frac{C_{g\phi} + U_{\phi}}{R}\right) \frac{\partial E}{\partial \phi} - \frac{(C_{g\phi} + U_{\phi})tan\phi}{R} E = SS(E)$$

Source functions

- $SS(E) = S_{in}$ Wind input source function
 - $+ S_{ds}$ Dissipation source function
 - $+ S_{bo}$ Bottom fraction source function
 - $+ S_{nl}$ Nonlinear interaction source function
 - + S_{cu} Current-wave interaction

✓ 5D problem = 2D geographic space + 2D spectrum space + 1D time

✓ Bottlenecks :

✓ Huge computation cost for source functions

✓ Data commutation due to propagation

 $E = E(K, \lambda, \phi, t)$ $\vec{K} = (k_{\lambda}, k_{\phi})$ $\vec{U} = (U_{\lambda}, U_{\phi})$ $\vec{C}_{g} = (C_{g\lambda}, C_{g\phi})$

) Wave-number spectrum Wave-number Background current Group velocity

✓ Fortran 90 + MPI

- ✓ Double precision
- ✓ Explicit numerical method

Evolution of MASNUM wave model

1990s	Early 2000s	Late 2000s	Early 2010s	Present
 LAGFD Serial Regional 	 MASNUM Serial Regional/ Global Coupled to OGCMs 	 MASNUM 128 cores in parallel (2007) Regional/ Global Coupled to OGCMs 	 MASNUM 130,000 cores (2014) Regional/ Global Coupled to OGCMs Coupled to ESM 	 MASNUM 10,649,60 0 cores (2016) Regional/ Global Coupled to OGCMs Coupled to ESM Ultra-high resolution

Milestone 1: Irregular quasi-rectangular domain decomposition (2014)

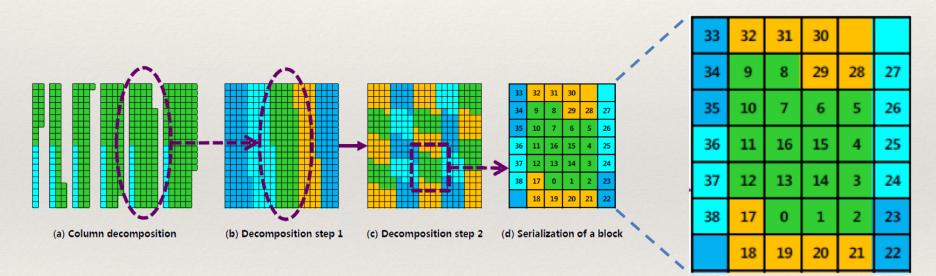


About 30% land points in global domain

Problem: In order to keep load balance, we should eliminate the land points.

Milestone 1: Irregular quasi-rectangular domain decomposition (2014)

An interesting mathematical game : Transforming a 2D plane into an 1D line.



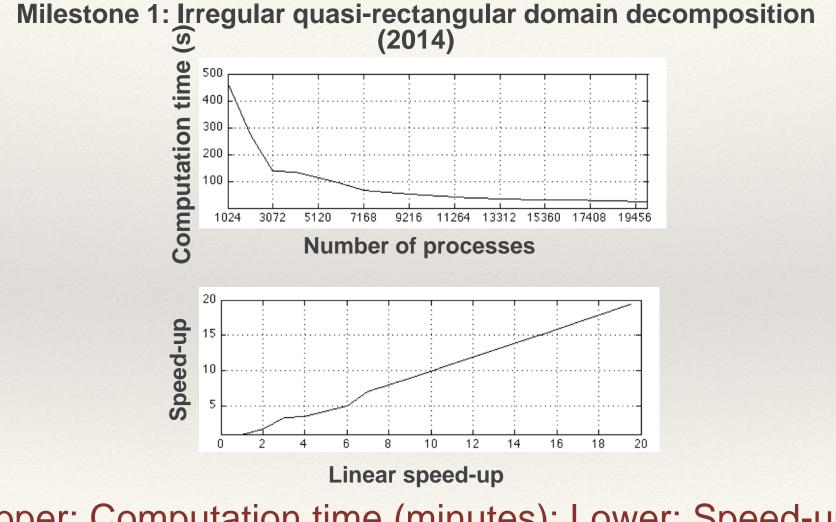
Comparing with the method of space filling curve, we keep the quasi-rectangular shape to simplify the implementation of communication and maintain good data locality.

Milestone 1: Irregular quasi-rectangular domain decomposition (2014)



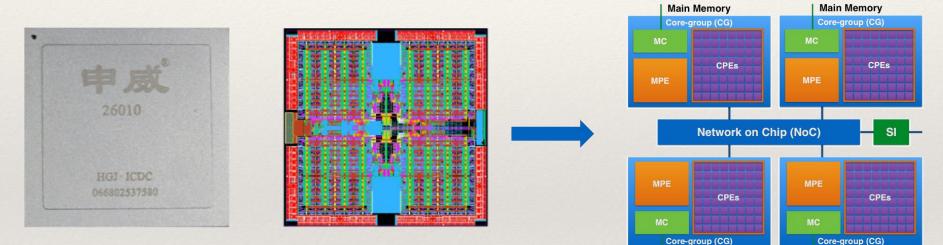
TIANHE-1A (National SuperComputer Center in Tianjin)

2* Intel Xeon X5670@2.93GHz + Tesla M2050						
24 GB/node						
RedHat						
Intel Compiler v12						
40 Gbps						



Upper: Computation time (minutes); Lower: Speed-up

Milestone 2: Master-slave cooperative computing workflow(2016)



SW26010 processors

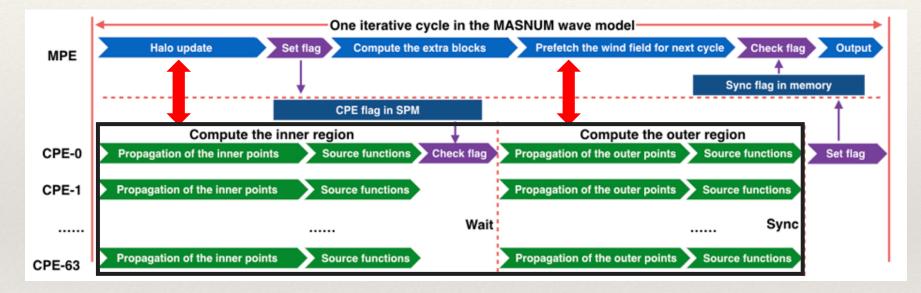
Main Memory

Main Memory

Sunway Taihulight Supercomputer



Milestone 2: Master-slave cooperative computing workflow(2016)

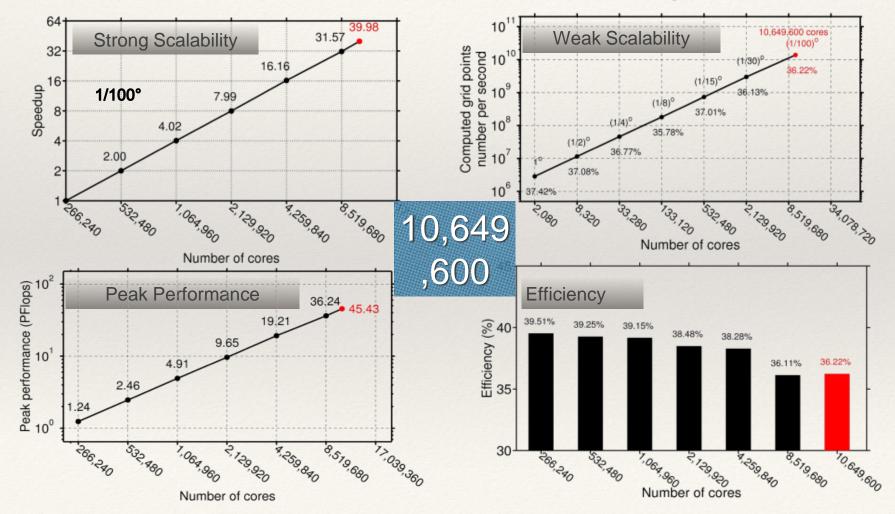


Cooperation: overlapping of communication and computing; data prefetching

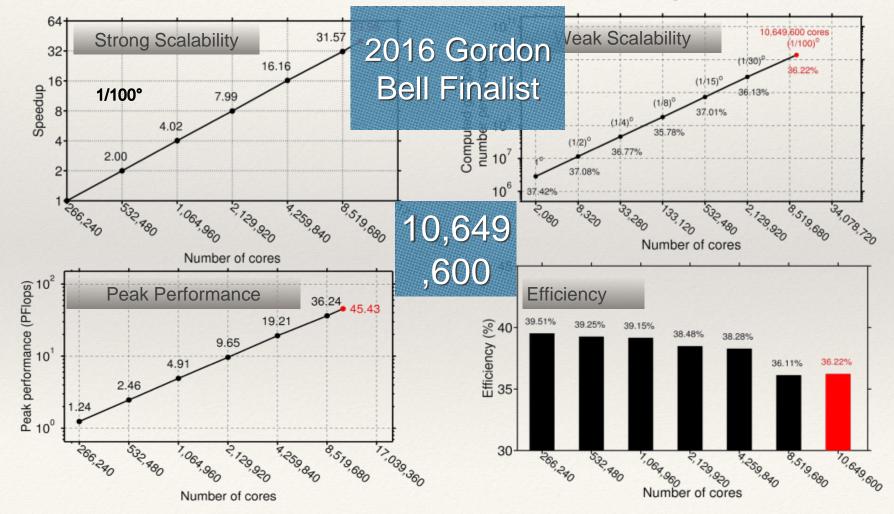
Synchronization : highly efficient synchronization among CPEs

Memory utilization: fully applied the local memory in CPEs (64KB)

Milestone 2: Master-slave cooperative computing workflow(2016)



Milestone 2: Master-slave cooperative computing workflow(2016)

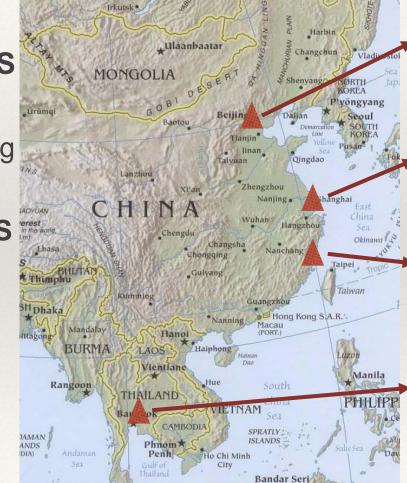


Operational forecasting system

OFS for ocean: Global Ocean Environment Forecasting Systems

1st generation OFS

- POM + MASNUM
- Assimilation: Nudging
- HR with 50 km
- o 2nd generation OFS
- MOM + SIS + MASNUM
- Assimilation: Ensemble adjust Kalman Filter
- HR with 10 km



National Marine Environment Forecasting Center, OFS2

East China Sea Marine Environment Forecasting Center, OFS1

Xiamen Marine Environment Forecasting Station, OFS1

UNESCO/IOC Ocean Forecasting demonstration System in the Southeast Asian Sea, OFS1

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Based on Code Modernization Optimization

Define the hotspots using Intel® VTune[™] Amplifier
Guarantee the load balance using Intel® Trace Analyzer & Collector

Optimized on Single Node

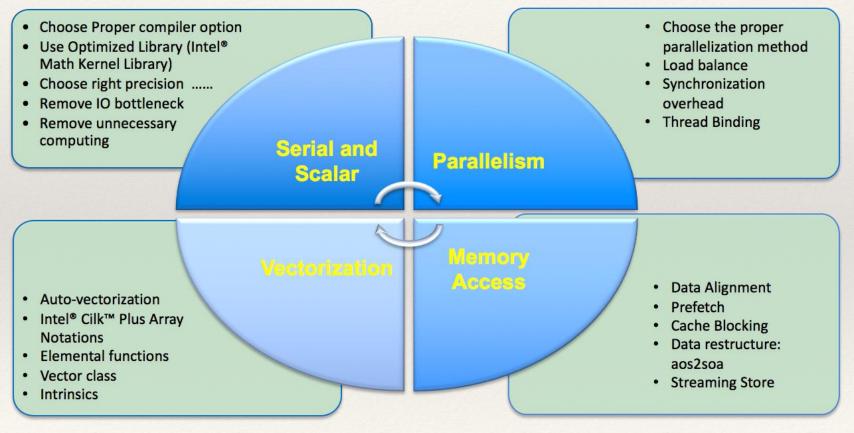
- Scalar optimization
- Vector optimization
- Improve Memory access Efficiency
- Fine-Grained Parallelism

Optimized on Cluster Level

• Extend the optimization to multi nodes

Optimization Methodology

Based on Code Modernization Optimization



Optimization Methodology

Optimization of MASNUM surface wave model on Xeon

	Xeon
CPU	Intel Xeon E5 2699 v3, 18 cores
amount	2 way in single node
Nodes	7 nodes, 252 cores in total
Frequency	2.3 GHz
Memory	128 GB
OS	RHEL 6.5
Compiler	Intel Compiler 16.0
MPI	Intel MPI 5.1.1

Based on Code Modernization Optimization

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 - Optimized on Single Node
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Optimized on Cluster Level

• Extend the optimization to multi nodes

Optimization Methodology

Step 1.1: Analysis Load-balance with ITAC

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Load-balance is good!

Step 1.2: Analysis Hotspots on Single node with Intel Vtune

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propagat preinf	444	ead2=-2.*sap*sam/al31				0.0%	0.0	0x5e0166		vmovsdq 0x1b8(%rsp), %xmm12	8.0%
svml sincos4	449	adm=ad/al23				0.0%		0x5e0174		vmulsd %xmm8, %xmm3, %xmm4	5.4%
	451	deladp=cwks17*(eij2/al11	,	al13		0.0%	0.0	0x5e01b4		movq 0x240(%rsp), %r11	4.7%
L_MPIintel_avx_rep_memcpy	455	se(kp2,j11)= se(kp2,j11)				0.0%	0.0	0x5e0115		movq 0xla0(%rsp), %rl0	4.7%
D_libm_exp_19	446	fcen=fconst0(k,idx)*enh(0.0%	0.0	0x5e010c		vdivsdq 0xla8(%rsp), %xmm10, %xmm0	
Ppmpi_bcast_	447	ad=cwks17*(eij2*ead1+ead				0.0%	0.0		444	vmulsd %xmm3, %xmm12, %xmm10	4.0%
	450	delad =cwks17*(eij*2.*ea	d1 sad2) *fcen			0.0%	0.0	0x5e0152		vmulsd %xmm9, %xmm12, %xmm9	3.6%
	611 452	eefab=min(eefab,deltee) deladm=cwks17*(eij2/al21	w team) the and	-122		0.0%	0.0	0x5e015c 0x5e3314		vmulsd %xmm8, %xmm15, %xmm0	1.9%
	452	sap=up+up1	- zu +sap) +rcen/a	at23		0.0%		0x5e3314 0x5e0144		<pre>vminpd %ymml2, %ymm0, %ymml2 vfmadd213sd %xmm0, %xmm14, %xmm15</pre>	1.5%
	433	eadl=sap/all1+sam/al21				0.0%	0.0	0x5e0144		vdivsd %xmm7, %xmm5, %xmm7	1.2%
	412	do j=1,jl				0.0%	0.0	0x5e01a5		vmovsdq (%r13), %xmm9	0.8%
	463	dse(ks ,js)=dse(ks ,js)-2. *delad			0.0%	0.0	0x5e033a		vmovsdq %xmm7, (%r15,%rax,1)	0.4%
	459	se(im ,j21)= se(im ,j21)				0.0%	0.0	0x5e0096		vmulsdq (%r14,%r12,1), %xmm3, %xmm	
	471	dse(im1,j22)=dse(im1,j22				0.0%	0.0	0x5e00c4		vaddsd %xmm2, %xmm2, %xmm12	0.4%
	460	se(im ,j22)= se(im ,j22)	+adm m12		0.8	0.0%	0.0	0x5e0280	460	vmovsdq %xmmll, (%r10,%r11,1)	0.4%
	461	se(im1,j21)= se(im1,j21)	+adm ^a m21		0.8	0.0%	0.0	0x5e01a0	452	vdivsd %xmm12, %xmm4, %xmm12	0.4%

implsch is the hotspot!

Based on Code Modernization Optimization

Define the hotspots using Intel® VTune™ Amplifier
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Optimized on Single Node

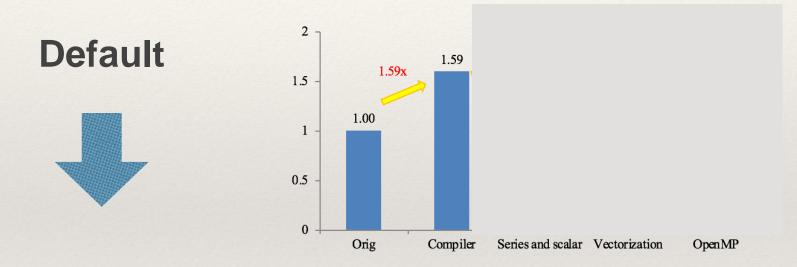
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Optimized on Cluster Level

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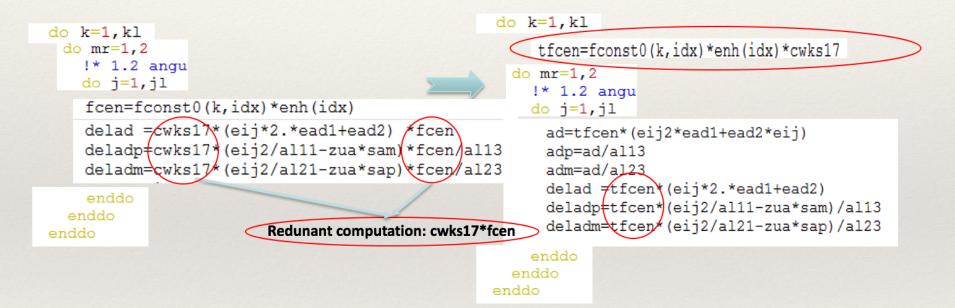
Optimization Methodology

Step 2.1: Best Compiler Option before optimized on Single Node



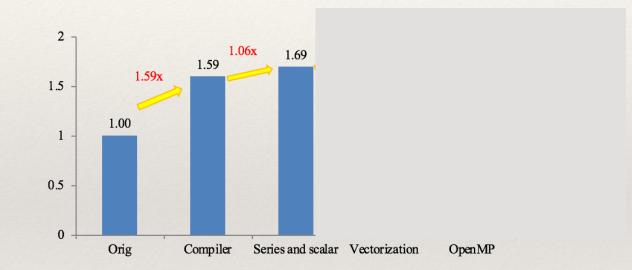
-O3 -xHost -align array32byte -no-prec-div

Step 2.2: Serial and Scalar Optimization



Reduce the redundant computations

Step 2.2: Serial and Scalar Optimization



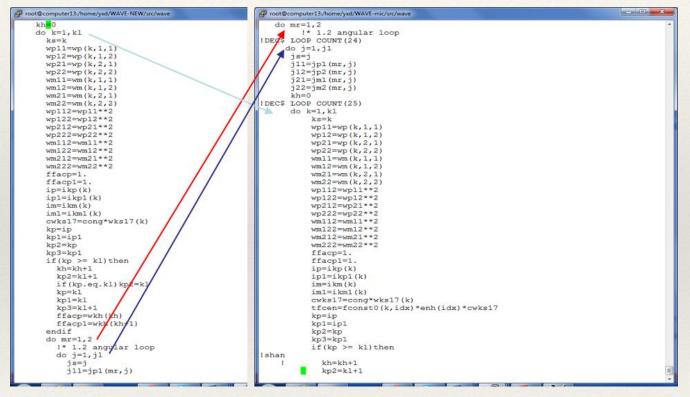
Reduce the redundant computations

Step 2.3: Vectorization Optimization

	410 411 412 413	<pre>do mr=1,2 !* 1.2 angular loop do j=1,j1 js=j</pre>
LOOP BEGIN at/src/wave/wamcor_mod.f90(410,7) remark #15344: loop was not vectorized: vector dependence prevents vec torization remark #15346: vector dependence: assumed OUTPUT dependence between wa	417	j11=jp1(mr,j) j12=jp2(mr,j) j21=jm1(mr,j) j22=jm2(mr,j)
mvar mod mp se line 454 and wamvar mod mp se line 462		
remark #15346: vector dependence: assumed OUTPUT dependence between wa mvar_mod_mp_se_ line 462 and wamvar_mod_mp_se_ line 454	447 448 449	ad=cwks17*(eij2*ead1+ead2*eij)*fcen adp=ad/al13 adm=ad/al23
LOOP BEGIN at/src/wave/wamcor_mod.f90(412,9) remark #15344: loop was not vectorized: vector dependence prevents vectorization	450 451 452	<pre>delad =cwks17*(eij*2.*ead1+ead2) *fcen deladp=cwks17*(eij2/al11-zua*sam)*fcen/al13 deladm=cwks17*(eij2/al21-zua*sap)*fcen/al23</pre>
remark #15346: vector dependence: assumed OUTPUT dependence between wamvar_mod_mp_se_ line 454 and wamvar_mod_mp_se_ line 462 remark #15346: vector dependence: assumed OUTPUT dependence between	454	<pre>se(ks , js) = se(ks , js) -2.0*ad se(kp2, j11) = se(kp2, j11) +adp*wp11</pre>
<pre>wamvar_mod_mp_se_ line 462 and wamvar_mod_mp_se_ line 454 LOOP END</pre>	456 457	se(kp2,j11) = se(kp2,j11)+adp*wp11 se(kp2,j12) = se(kp2,j12)+adp*wp12 se(kp3,j11) = se(kp3,j11)+adp*wp21
	458 459 460	<pre>se(kp3,j12) = se(kp3,j12) + adp*wp22 se(im, j21) = se(im, j21) + adm*wm11 se(im, j22) = se(im, j22) + adm*vm12</pre>
	461 462	<pre>se(im ,j22)= se(im ,j22)+adm*wm12 se(im1,j21)= se(im1,j21)+adm*wm21 se(im1,j22)= se(im1,j22)+adm*wm22</pre>

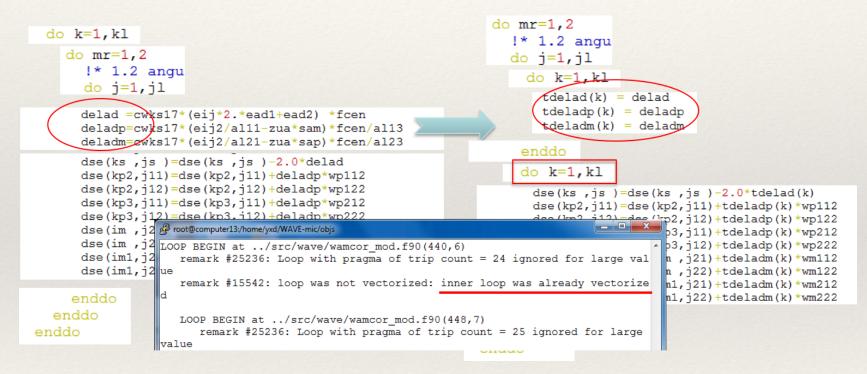
Analyze by using compiler option "-qopt-report=5"

Step 2.3: Vectorization Optimization



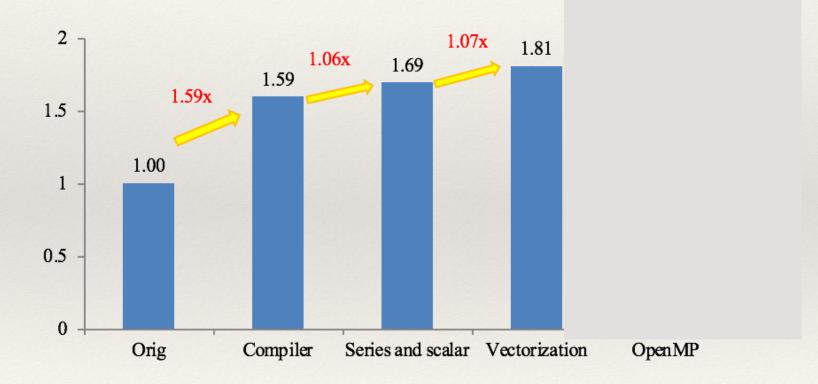
Exchange the Loop sequence

Step 2.3: Vectorization Optimization



Remove the dependence

Step 2.3: Vectorization Optimization



Step 2.4: Fine-Grained Parallelism

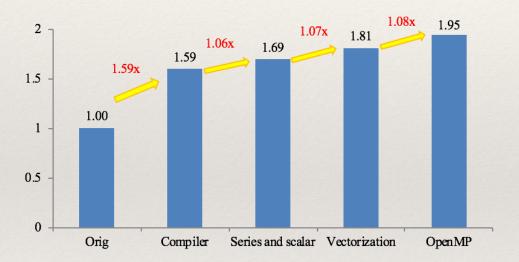
SOMP PARALLELDO PRIVATE (idx)

do idx=1,np call mean2(idx) enddo

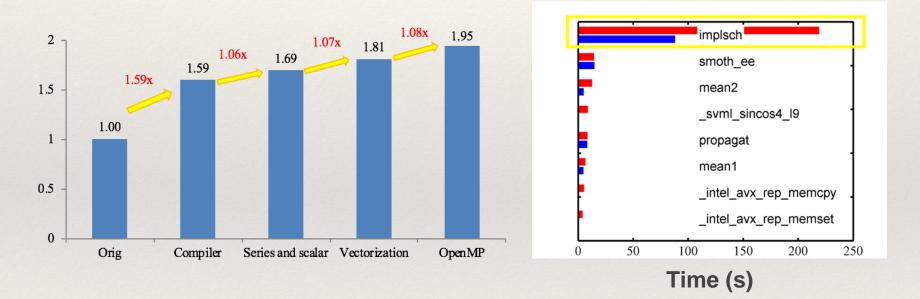
```
allocate(tad(klp1))
   allocate(tadp(klp1))
   allocate(tadm(klp1))
   allocate(tdelad(klp1))
   allocate(tdeladm(klp1))
   allocate(tdeladp(klp1))
   allocate(tkh(klp1))
!SOMP PARALLELDO DEFAULT (NONE) SHARED (pein, peds, pebo, nsp, awk, wx, wy) &
!$OMP SHARED(kpmt0, kakt0, fconst0, wf, d, enh, e, ee, w, ks0) &
!$OMP SHARED(wk,ikp,jp1,jp2,jm1,jm2,wp,wm,ikp1,ikm,ikm1,wks17)&
!$OMP SHARED(wkh,tkh,presin,precos,grolim)&
!$OMP SHARED(awf,asi,ark,ae,uxx,uxy,uyx,uyy,ccg)&
!$OMP SHARED(cong,np,alog10pwk,al31,al11,al12,al21,al13,al23,dwk,deltt,deltt5)
$
!SOMP PRIVATE(awkss, vx, vy, ww, wkpm, wkpmt, wakt, beta) &
!$OMP PRIVATE(xx,wp11,wp12,wp21,wp22,wm11,wm12,wm21,wm22)&
SOMP PRIVATE (wp112, wp122, wp212, wp222, wm112, wm122, wm212, wm222, ffacp, ffacp1) &
!$OMP PRIVATE(cwks17,rij,eij,ea1,ea2,ea3,ea4,ea5,ea6,ea7,ea8,up,up1)&
!SOMP PRIVATE(um,um1,sap,sam,eij2,zua,ead1,ead2,fcen,ad,adp,adm,delad)&
!$OMP PRIVATE(deladm,cd,theta0,costh,sinth,wl,wlstar,wk0,wf0,ws0,bett)&
!$OMP PRIVATE(awfss,arkss,aess,eks,ekspm,sds,asiss,ssds,d0,dk,ssbo,duxdx0) &
SOMP PRIVATE (duydx0, duydy0, th0, cost2, sint2, cq, cp, cqdc, cu1, cu2, cu3, sscu) &
!SOMP PRIVATE(wstar,deltee,eef,gadiag,eefab,sig,deladp,duxdy0,sbo)&
!$OMP PRIVATE(kpmt, kakt, ks1, ks, ksp1, k, j, kh, ip, ip1, im, im1) &
!$OMP PRIVATE(kp, kp1, kp2, kp3, mr, js, j11, j12, j21, j22, i) &
!$OMP PRIVATE(tfcen, tasds, tad, tadm, tadp, tdeladp, tdeladm, tdelad) & !shan
!$OMP PRIVATE(se,dse,sein,seds,sebo SCHEDULE(GUIDED,7)
```

use Open MP "!\$OMP PARALLELDO" for parallelization

Step 2.4: Fine-Grained Parallism



Step 2.4: Fine-Grained Parallism



Based on Code Modernization Optimization

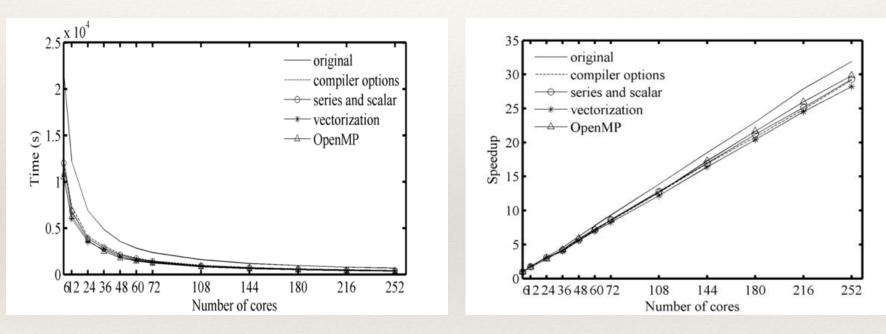
- Define the hotspots using Intel® VTune™ Amplifier
 Guarantee the load balance using Intel® Trace Analyzer & Collector
 - Optimized on Single Node
 - Scalar optimization
 - Vector optimization
 - Improve Memory access Efficiency
 - Fine-Grained Parallelism

Optimized on Cluster Level

• Extend the optimization to multi nodes

Optimization Methodology

Step 3: Optimization on multi-nodes



Execution times before and after optimization

Scalability before and after optimization

Outline

- Brief Introduction of Intel[®] PCC at FIO
- Background
- Optimization strategy
- Future work

Future work

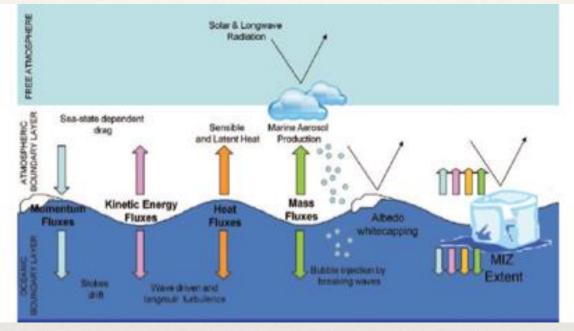
- Optimize on the new Intel Architecture (wider vector length)
- Optimize the MASNUM surface wave model on large-scale cluster
- Try to apply the optimization strategy to other ocean and atmosphere models

THANK FOR YOUR ATTENTION

Contact: songroy@fio.org.cn

Coupled models by incorporated ocean surface wave model

Importance of ocean surface wave

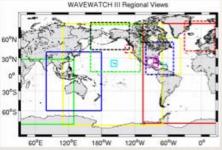


- Ocean surface wave is also important in the ocean and climate system.
- Coupled with ocean surface wave model is a way to accurate simulating and forecasting for ocean and climate

Intel[®] PCC at FIO

T1: Model computing performance—simulating faster

NCEP (USA), 60^{°N} WaveWatch III 0° Global: 1.25 x 1.00° Region: 0.25 x 0.25° 6°s

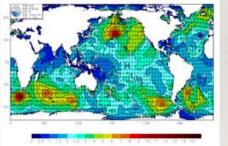


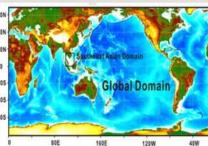


ECMWF (Europe), WAM, Global 7-day: 0.125 x 0.125° 15-day: 0.25 x 0.25°

State-of-the-art of wave forecasting

NMEFC (China), SWAM Global: 0.5 x 0.5° Region: 0.125 x 0.125°





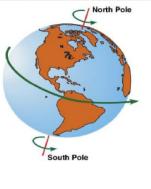
IOC/WESTPAC, MASNUM Global: 0.5 x 0.5° Region: 0.125 x 0.125°

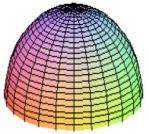


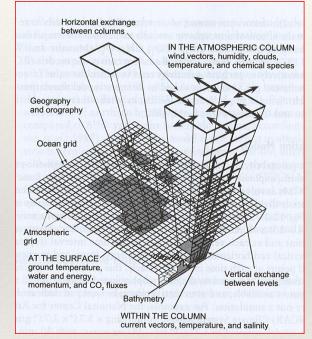
7-days forecasting within 90 minutes Resolution finer, simulation ability better Fine-resolution is still a challenge

Intel[®] PCC at FIO

T2: Model simulation ability—more accurate







Parameterizatio n: unsolved physical process due to resolution

 Model tuning: a hard work, depending on modeler empirically
 Parameter optimization: by using deep learning