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Strategy of the code modernization optimization for ocean numerical model: A case study of MASNUM wave model

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+ Intel® Parallel Computing Center at FIO

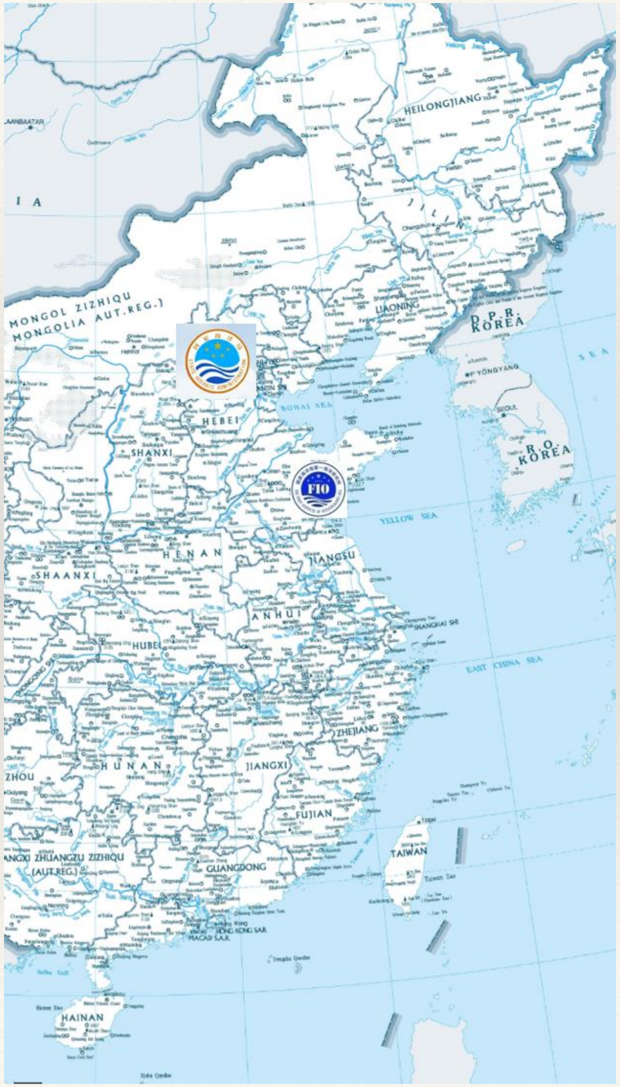
Outline

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

Introduction of FIO

- MNR Headquarters, Beijing
- 4 Research Institute
  - **FIO, Qingdao**
  - SIO, Hangzhou
  - TIO, Xiamen
  - 4IO, Beihai (being built)

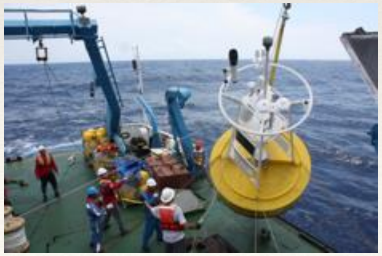
- 8 Operational Centers
  - NMEFC, NMEMC, NMDIS…
- 3 Branches
  - North Sea, East Sea, South Sea

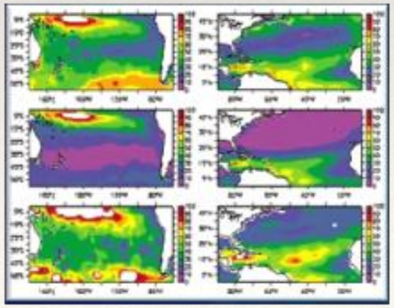


Introduction of FIO

Mission

- Basic and applied research in oceanography, marine science and technology.
- Technical support and research service to the development of high-tech 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.





Introduction of FIO

Structure

- Director General
  - Vice DGs
    - MASNUM
      - Lab of Marine Science and Numerical Modeling
      - Lab of Marine Geology and Geophysics
      - Lab of Marine Physics and Remote Sensing
      - Ocean and Climate Research Center
      - Marine Ecology Research Center
      - Research Center for Island &Coastal Zone
      - Marine Engineering Environment & Geomatic Center
    - HPCC
      - Marine Information and Data Center
      - High-performance Computing Center
      - Library
      - China Ocean Sample Repository
      - Vessel Management Center
    - China-Korea Joint Ocean Research Center
    - China-Indonesia Ocean and Climate Center
    - China–Thailand Joint Laboratory for Climate and Marine Ecosystem
    - China–Australia Center for Marine Engineering
    - FIO-POI Joint Research Center For Ocean and Climate
    - FIO-UM Joint Center Of Marine Science and Technology
    - UNESCO/IOC Regional Training/Research Center on Ocean Dynamic & Climate
    - CLIVAR ICGPO
    - China-PEMSEA Sustainable Coastal Management Cooperation Center

Introduction of FIO

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


Zhenya Song


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

Outline

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Ocean surface wave model

Ocean surface wave

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

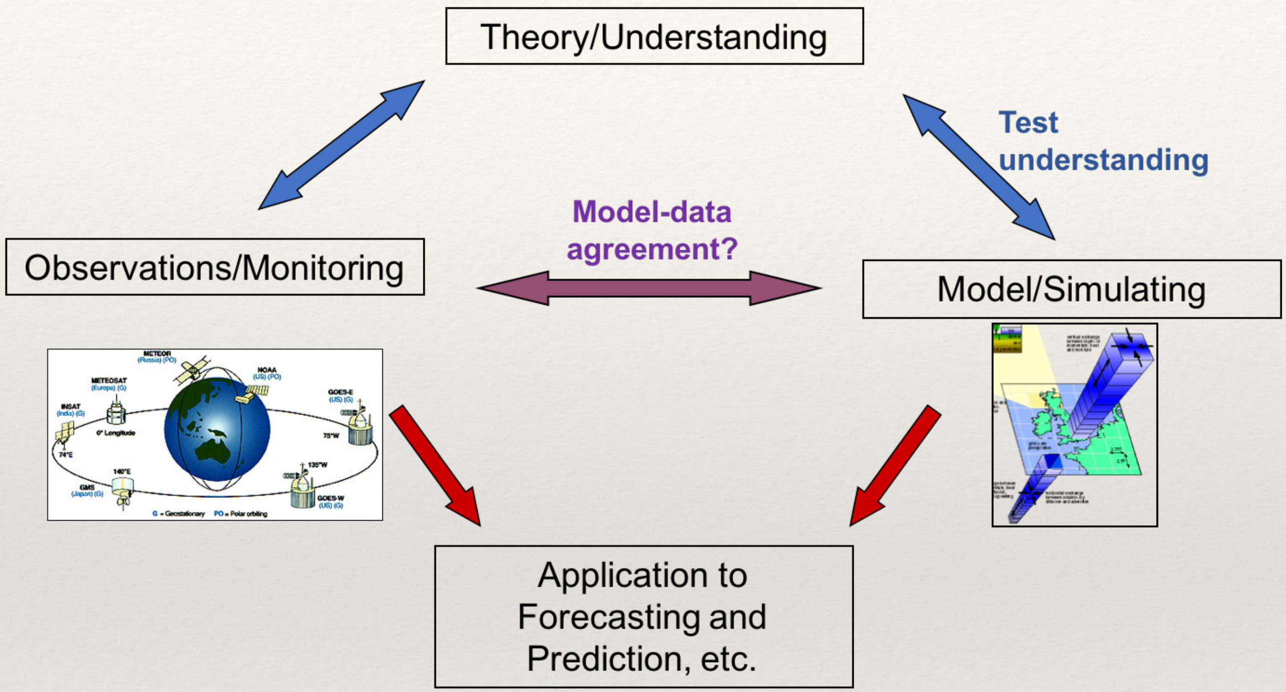
Ocean surface wave model

Importance of ocean surface wave




- Ocean surface wave is important for navigation.
- Ocean surface wave is important for ocean engineering

Ocean surface wave model

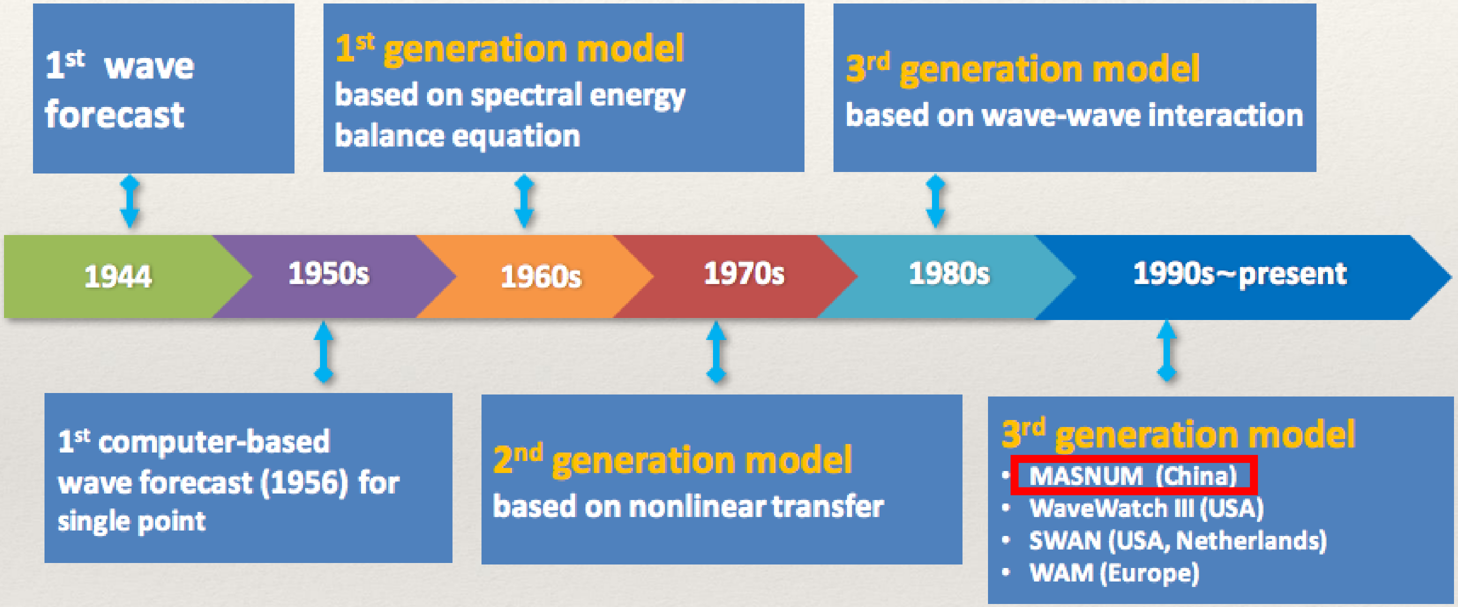


- Three methods: Theoretical research, Lab experiments and Observation, and Numerical simulation
- Model is the key tool for forecasting and prediction

Ocean surface wave model

History of ocean surface wave model

World War II



- 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

Ocean surface wave model

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

$E = E(K, \lambda, \phi, t)$ **Wave-number spectrum**
$\vec{K} = (k_{\lambda}, k_{\phi})$ **Wave-number**
$\vec{U} = (U_{\lambda}, U_{\phi})$ **Background current**
$\vec{C}_g = (C_{g\lambda}, C_{g\phi})$ **Group velocity**

- ✓ **5D problem = 2D geographic space + 2D spectrum space + 1D time**
- ✓ **Bottlenecks :**
  - ✓ **Huge computation cost for source functions**
  - ✓ **Data commutation due to propagation**

- ✓ **Fortran 90 + MPI**
- ✓ **Double precision**
- ✓ **Explicit numerical method**

Ocean surface wave model

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 • 10,649,600 cores (2016) • Regional/ Global • Coupled to OGCMs • Coupled to ESM • Ultra-high resolution

Ocean surface wave model

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

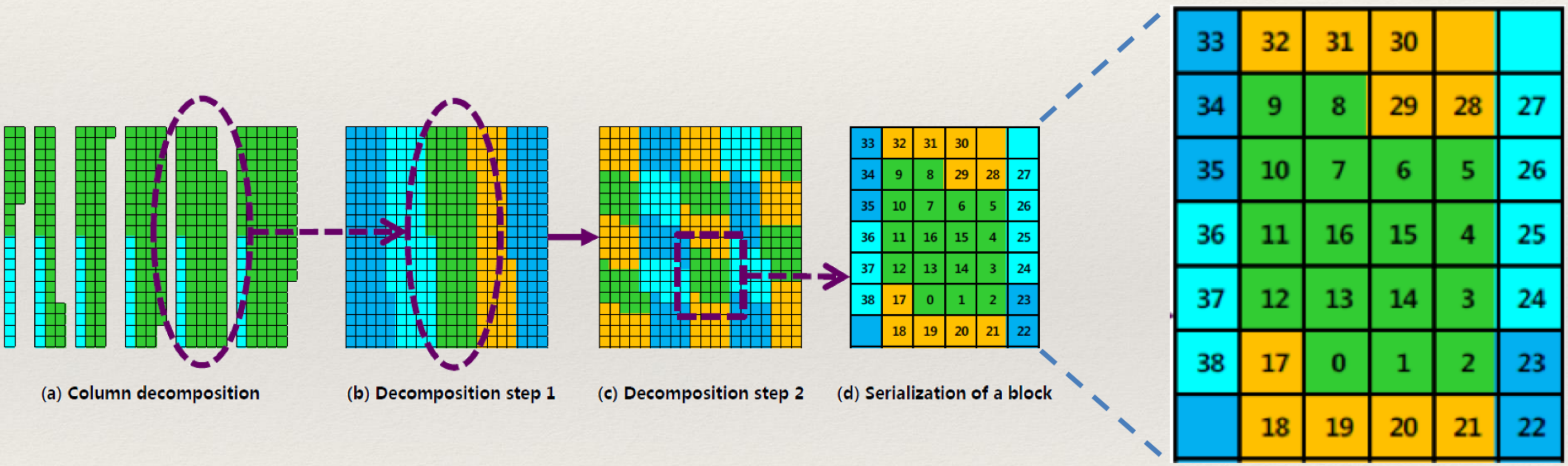
About 30% land points in global domain

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

Ocean surface wave model

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

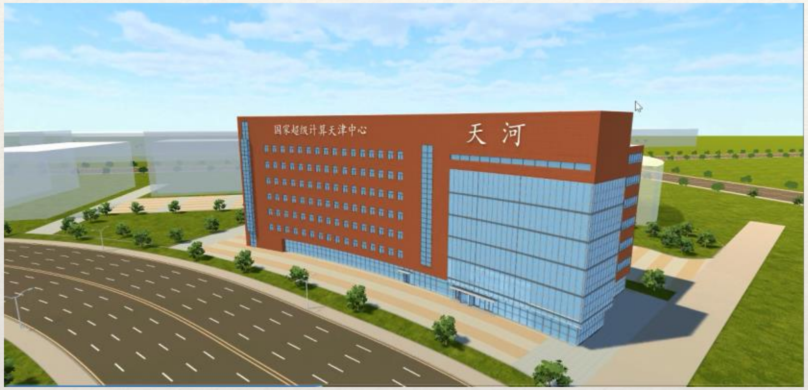
An interesting mathematical game : Transforming a 2D plane into an 1D line.



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.

Ocean surface wave model

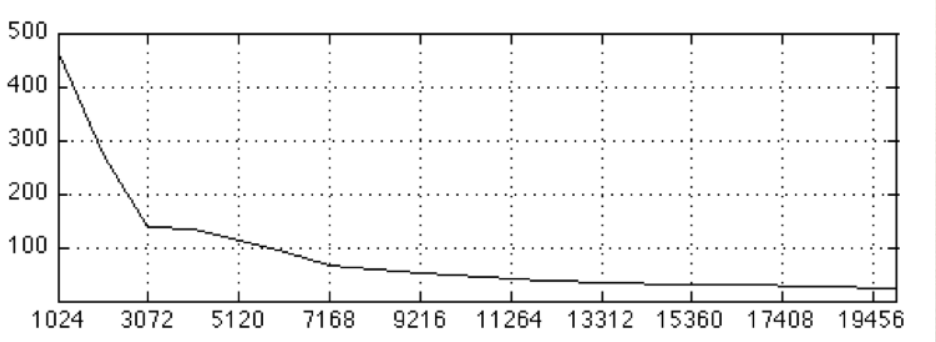
Milestone 1: Irregular quasi-rectangular domain decomposition (2014)

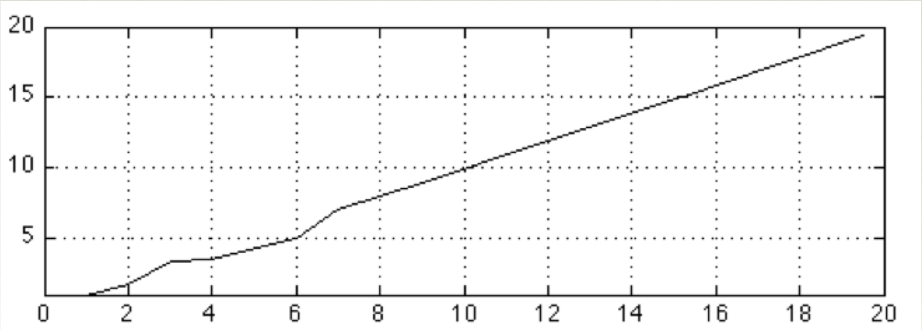


TIANHE-1A (National SuperComputer Center in Tianjin)	
CPU	2* Intel Xeon X5670@2.93GHz + Tesla M2050
Memory	24 GB/node
OS	RedHat
Fortran/C Compiler	Intel Compiler v12
MPI	
Network	40 Gbps

Ocean surface wave model

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

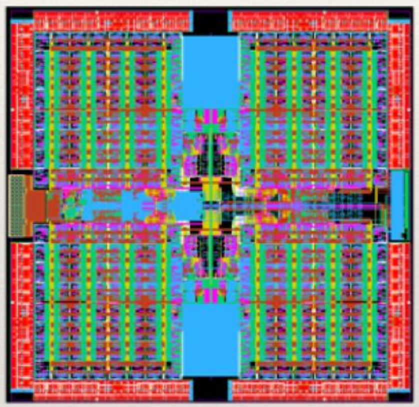




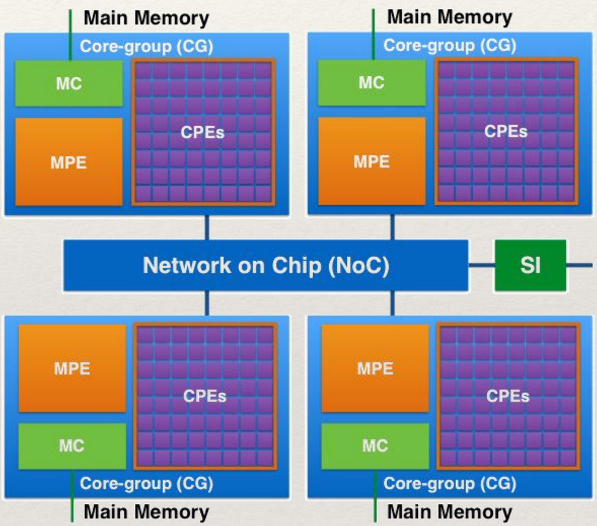
Upper: Computation time (minutes); Lower: Speed-up

Ocean surface wave model

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



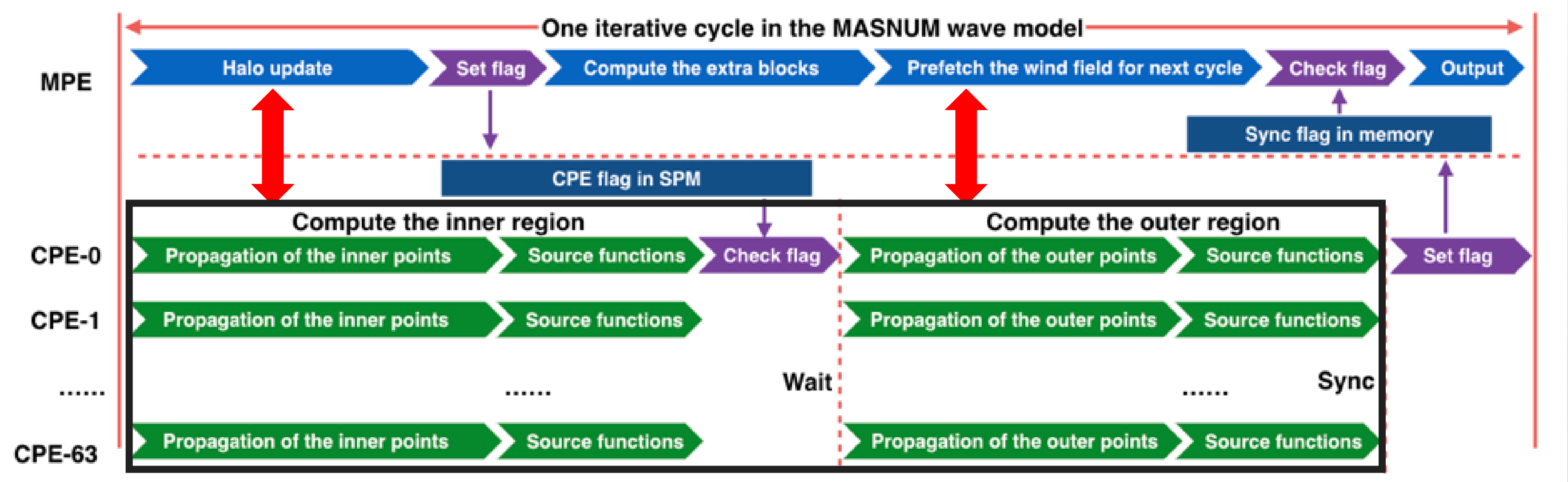
SW26010 processors



Sunway Taihulight Supercomputer

Ocean surface wave model

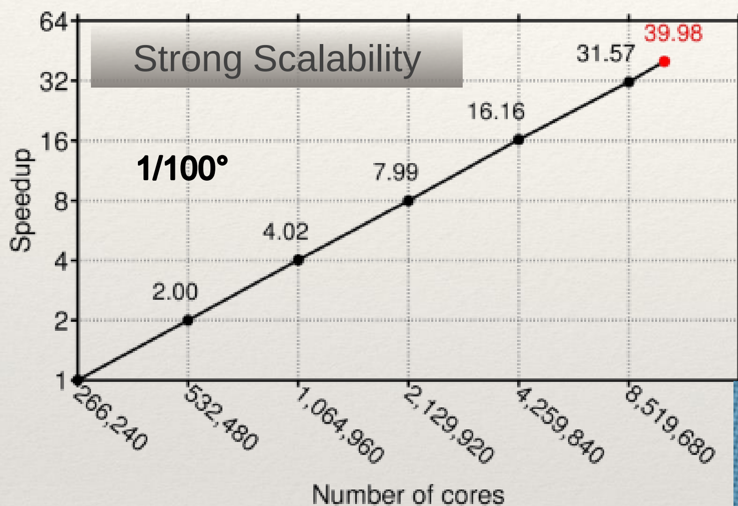
Milestone 2: Master-slave cooperative computing workflow(2016)

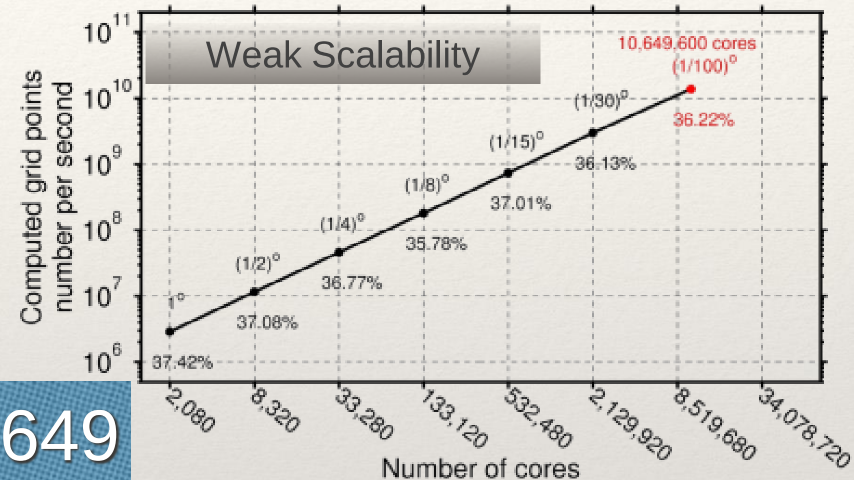


- **Cooperation**: overlapping of communication and computing; data prefetching
- **Synchronization** : highly efficient synchronization among CPEs
- **Memory utilization**: fully applied the local memory in CPEs (64KB)

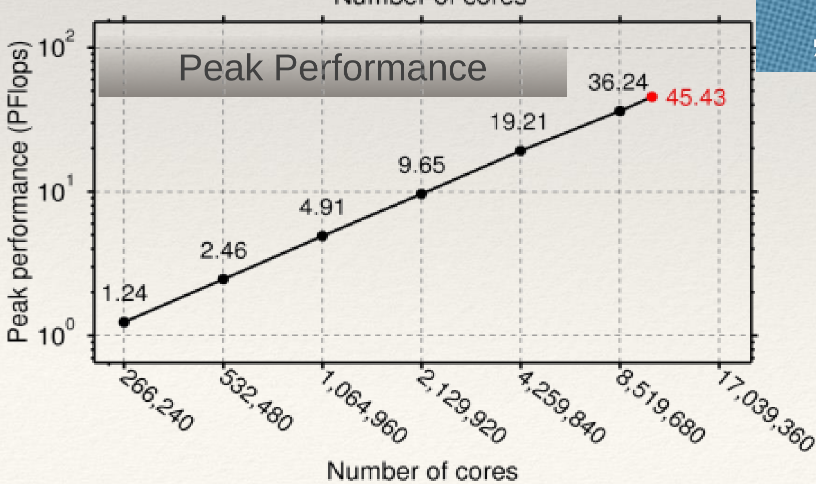
Ocean surface wave model

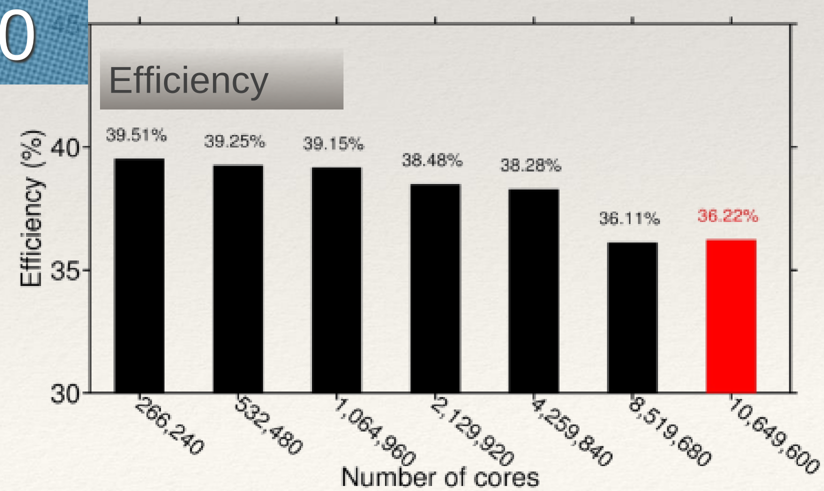
Milestone 2: Master-slave cooperative computing workflow(2016)





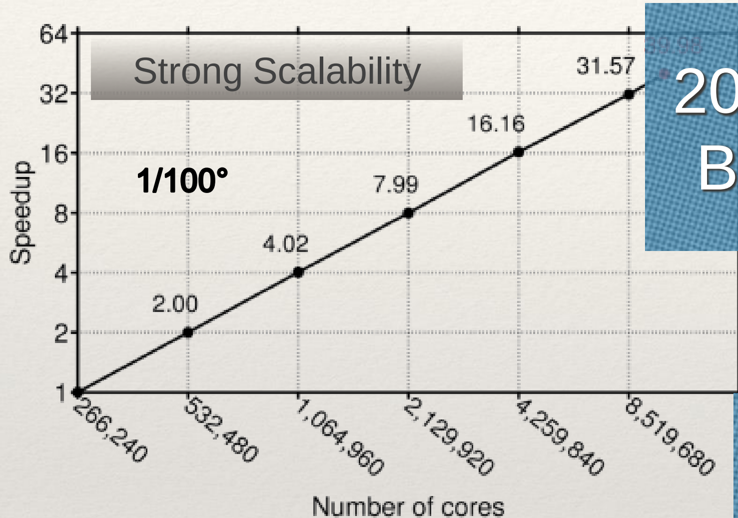
10,649
,600



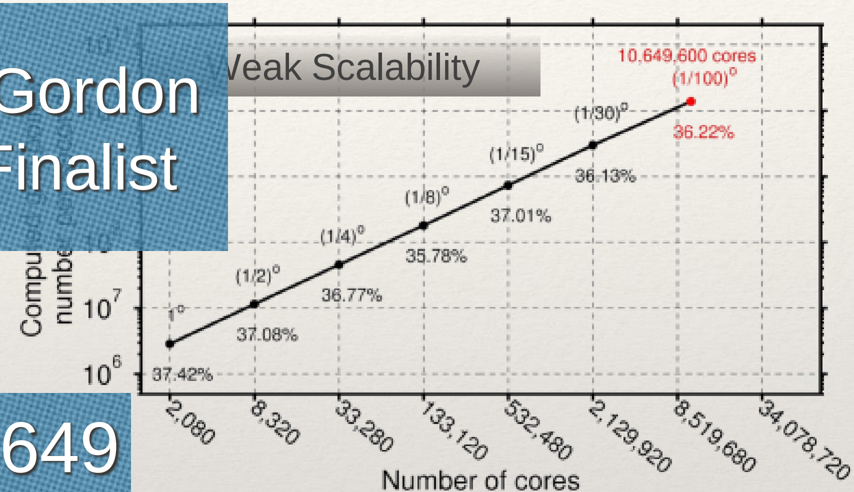


Ocean surface wave model

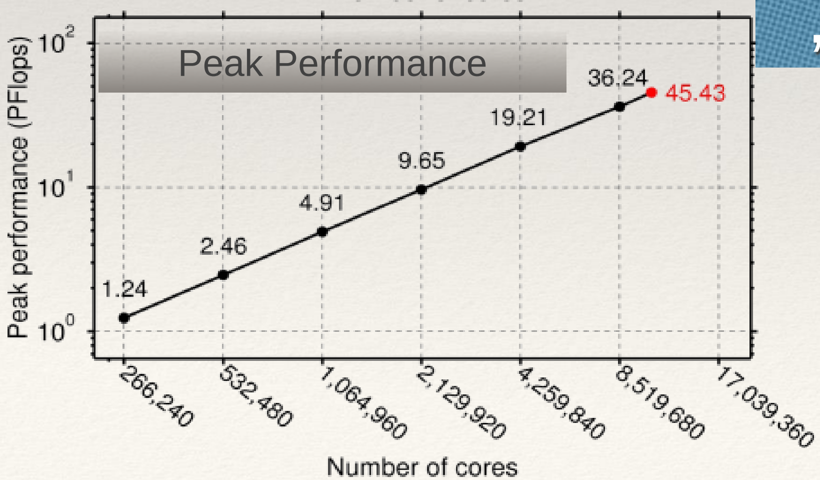
Milestone 2: Master-slave cooperative computing workflow(2016)

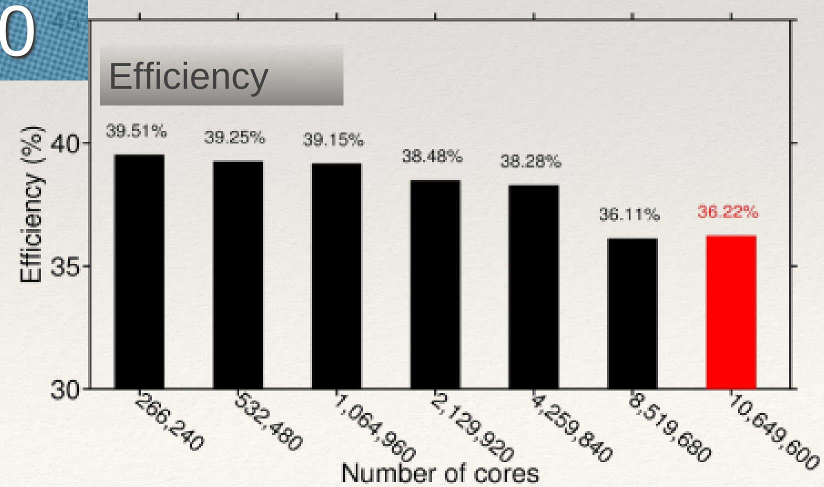


2016 Gordon Bell Finalist



10,649
,600





Operational forecasting system

OFS for ocean: Global Ocean Environment Forecasting Systems

- **1st generation OFS**
  - POM + MASNUM
  - Assimilation: Nudging
  - HR with 50 km
- **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

Outline

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- Future work

Optimization strategy

Based on Code Modernization Optimization

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

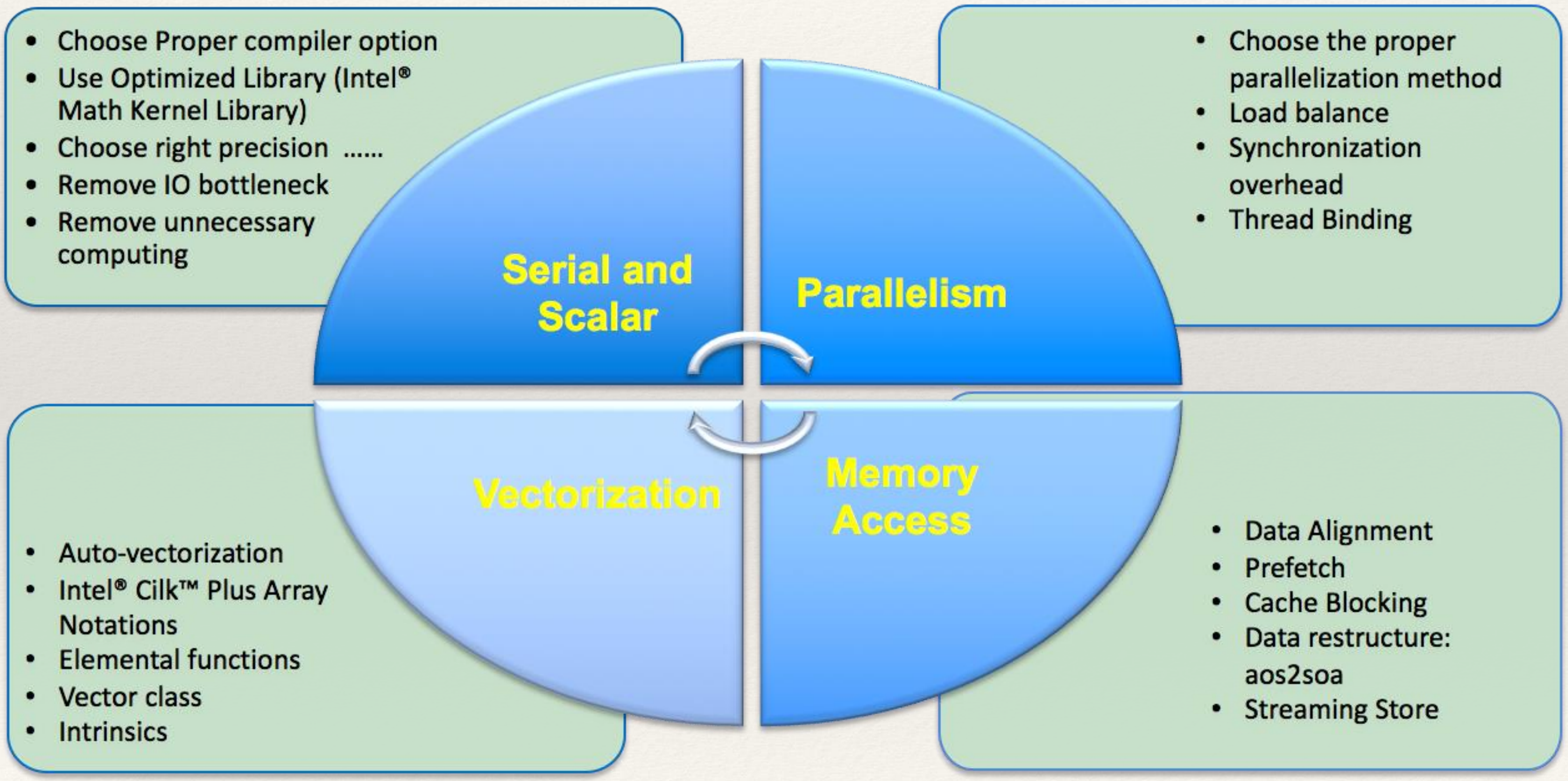
- Optimized on Single Node
  - Scalar optimization
  - Vector optimization
  - Improve Memory access Efficiency
  - Fine-Grained Parallelism

- Optimized on Cluster Level
  - Extend the optimization to multi nodes

Optimization Methodology

Optimization strategy

Based on Code Modernization Optimization



Optimization Methodology

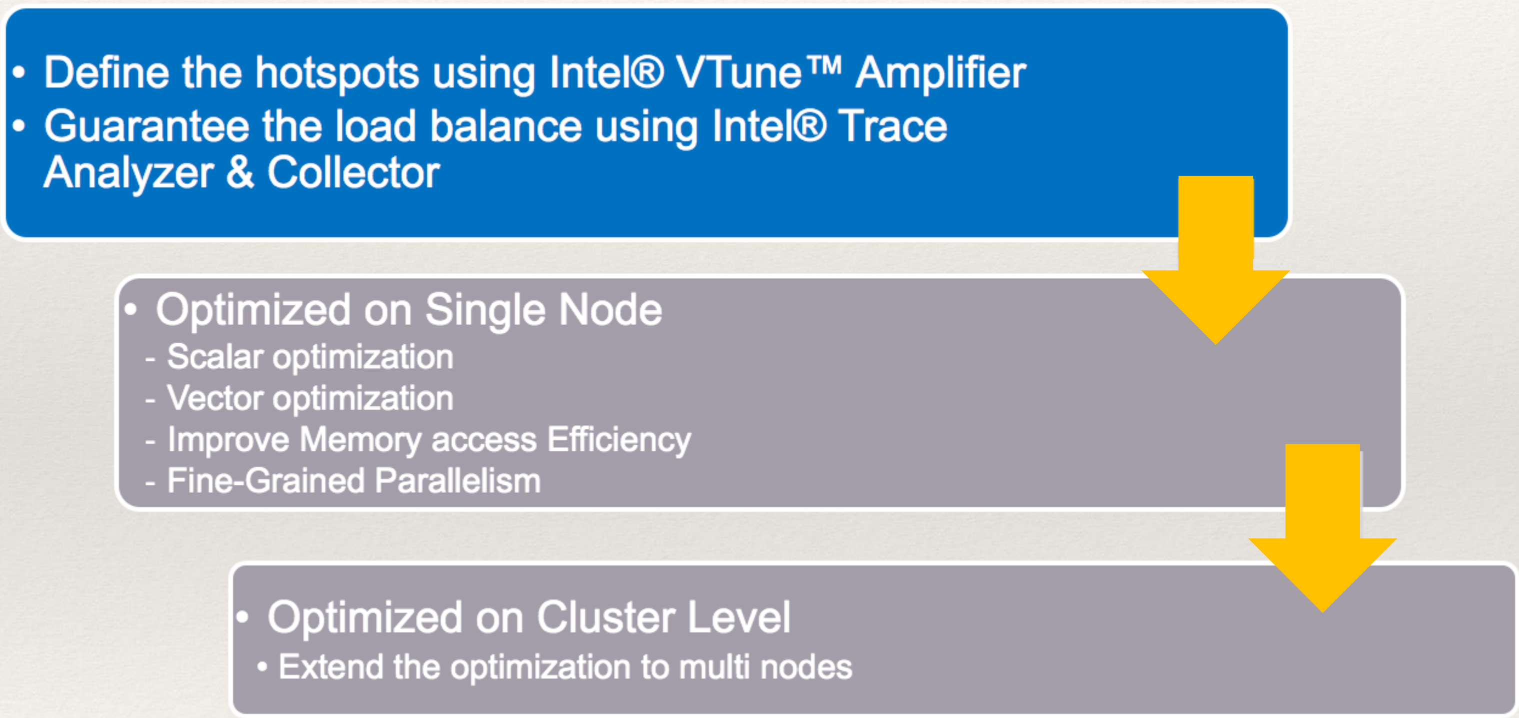
Optimization strategy

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

Optimization strategy

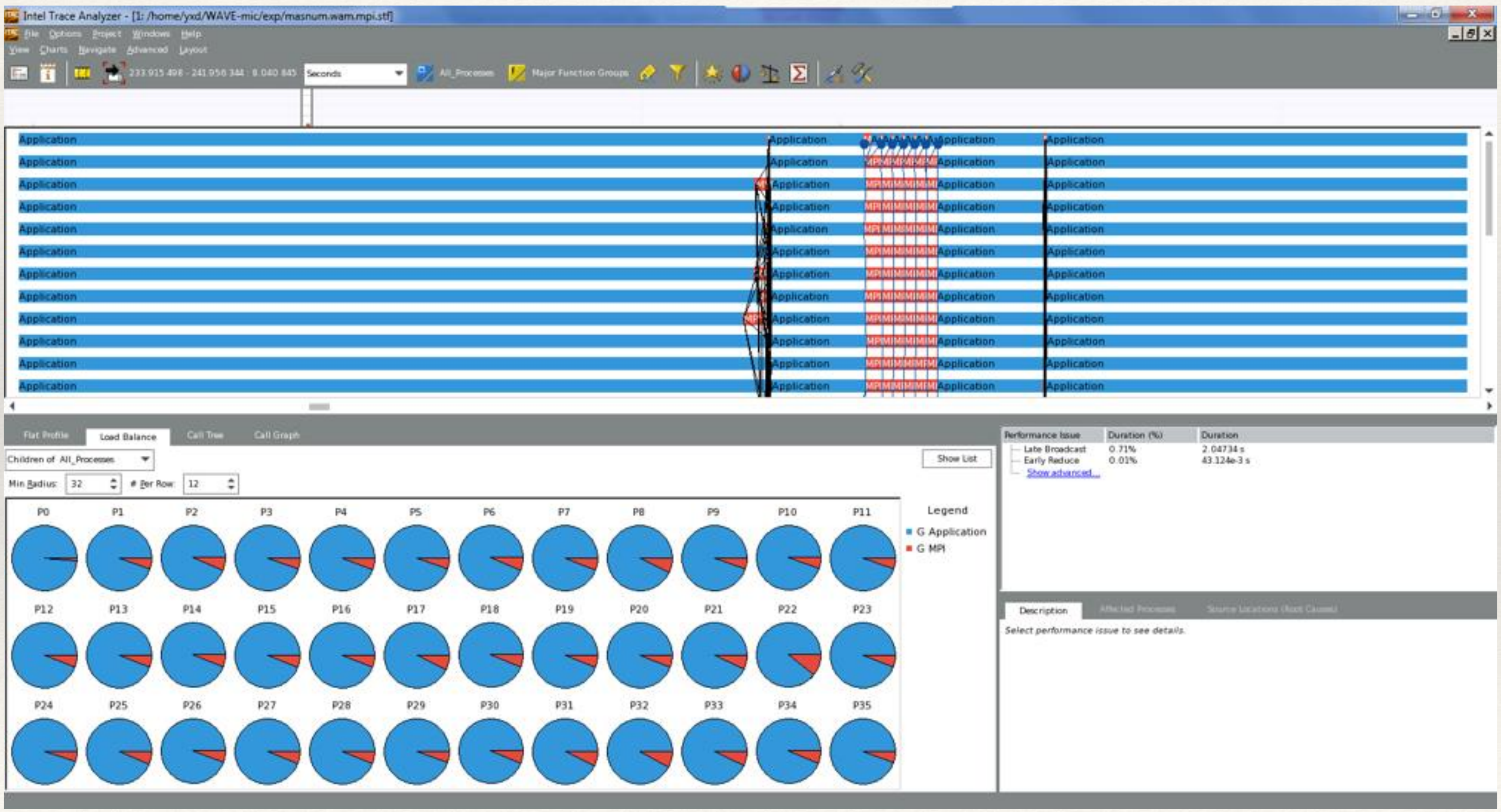
Based on Code Modernization Optimization



Optimization Methodology

Optimization strategy

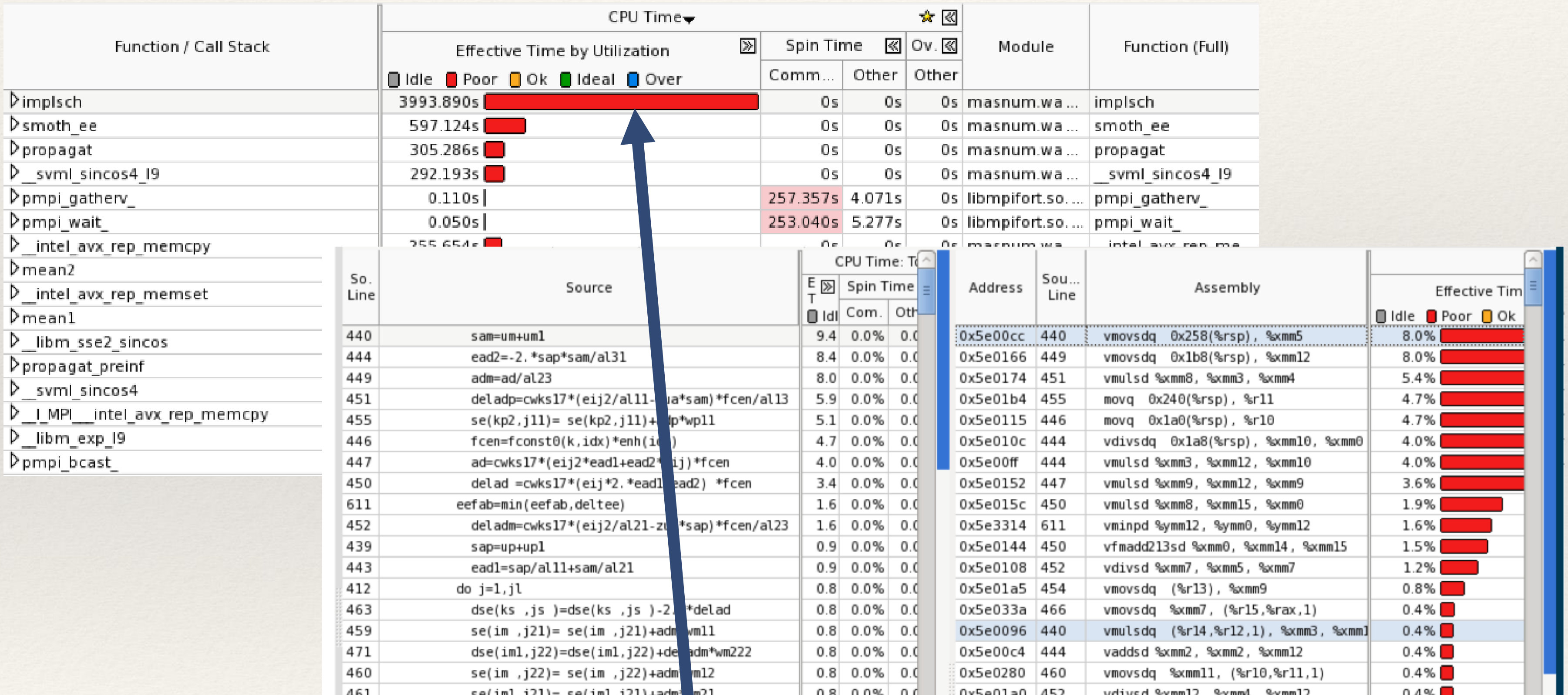
Step 1.1: Analysis Load-balance with ITAC



Load-balance is good!

Optimization strategy

Step 1.2: Analysis Hotspots on Single node with Intel Vtune



implsch **is the hotspot!**

Optimization strategy

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

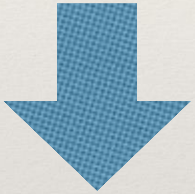
- Optimized on Cluster Level
  - Extend the optimization to multi nodes

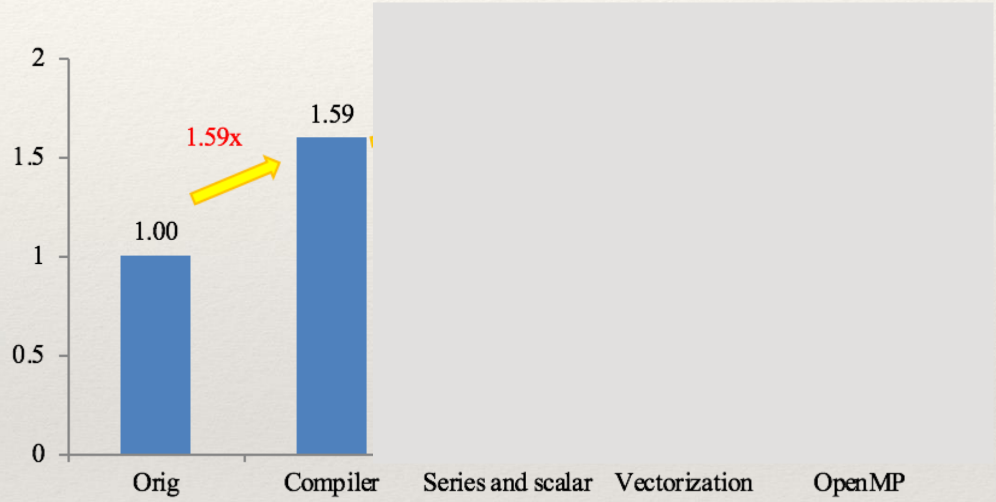
Optimization Methodology

Optimization strategy

Step 2.1: Best Compiler Option before optimized on Single Node

Default





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

Optimization strategy

Step 2.2: Serial and Scalar Optimization

```
do  k=1,kl
  do mr=1,2
    !* 1.2 angu
    do j=1,jl
     fcen=fconst0(k,idx)*enh(idx)
     delad =cwks17*(eij*2.*ead1+ead2) *fcen
     deladp=cwks17*(eij2/al11-zua*sam)*fcen/al13
     deladm=cwks17*(eij2/al21-zua*sap)*fcen/al23
    enddo
  enddo
enddo
```

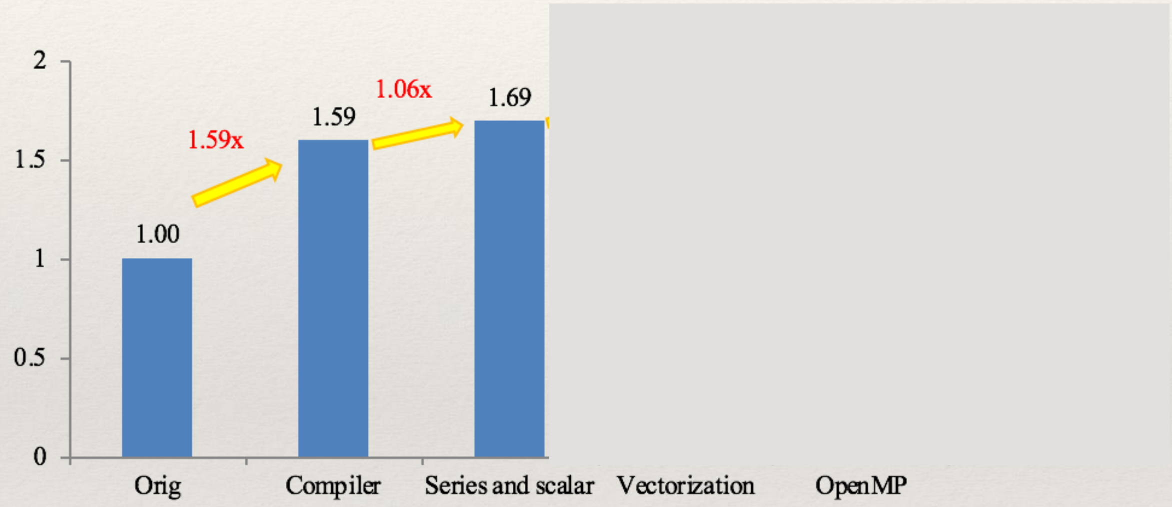
Redunant computation: cwks17*fcen

```
do  k=1,kl
  tfcen=fconst0(k,idx)*enh(idx)*cwks17
  do mr=1,2
    !* 1.2 angu
    do j=1,jl
      ad=tfcen*(eij2*ead1+ead2*eij)
      adp=ad/al13
      adm=ad/al23
      delad =tfcen*(eij*2.*ead1+ead2)
      deladp=tfcen*(eij2/al11-zua*sam)/al13
      deladm=tfcen*(eij2/al21-zua*sap)/al23
    enddo
  enddo
enddo
```

Reduce the redundant computations

Optimization strategy

Step 2.2: Serial and Scalar Optimization



Reduce the redundant computations

Optimization strategy

Step 2.3: Vectorization Optimization

```
   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
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

      LOOP BEGIN at ../src/wave/wamcor_mod.f90(412,9)
         remark #15344: loop was not vectorized: vector dependence prevents
vectorization
         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
 wamvar_mod_mp_se_ line 462 and wamvar_mod_mp_se_ line 454
      LOOP END
   LOOP END
LOOP END
```

```
410        do mr=1,2
411          !* 1.2 angular loop
412          do j=1,jl
413            js=j
414            j11=jp1(mr,j)
415            j12=jp2(mr,j)
416            j21=jm1(mr,j)
417            j22=jm2(mr,j)
```

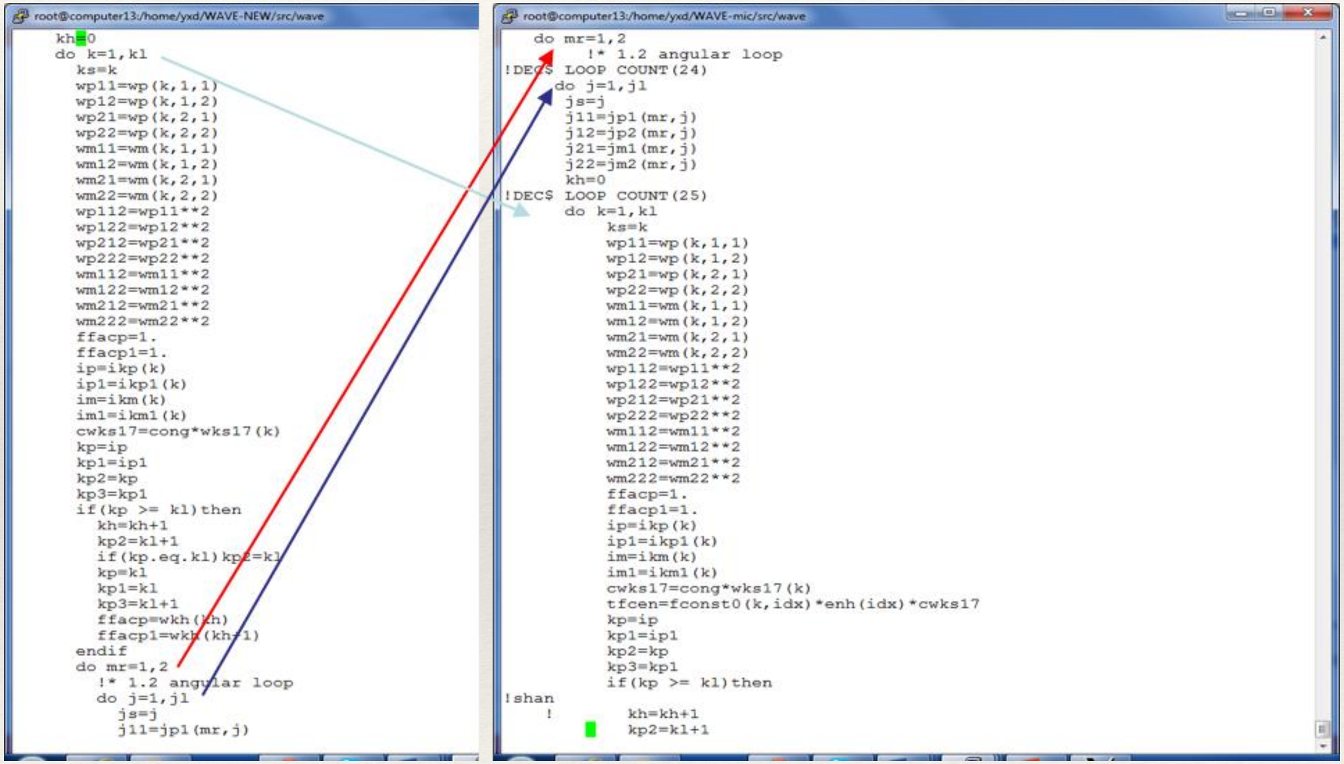
```
447            ad=cwks17*(eij2*ead1+ead2*eij)*fcen
448            adp=ad/al13
449            adm=ad/al23
450            delad =cwks17*(eij*2.*ead1+ead2) *fcen
451            deladp=cwks17*(eij2/al11-zua*sam)*fcen/al13
452            deladm=cwks17*(eij2/al21-zua*sap)*fcen/al23
```

```
454            se(ks ,js )= se(ks ,js )-2.0*ad
455            se(kp2,j11)= se(kp2,j11)+adp*wp11
456            se(kp2,j12)= se(kp2,j12)+adp*wp12
457            se(kp3,j11)= se(kp3,j11)+adp*wp21
458            se(kp3,j12)= se(kp3,j12)+adp*wp22
459            se(im ,j21)= se(im ,j21)+adm*wm11
460            se(im ,j22)= se(im ,j22)+adm*wm12
461            se(im1,j21)= se(im1,j21)+adm*wm21
462            se(im1,j22)= se(im1,j22)+adm*wm22
```

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

Optimization strategy

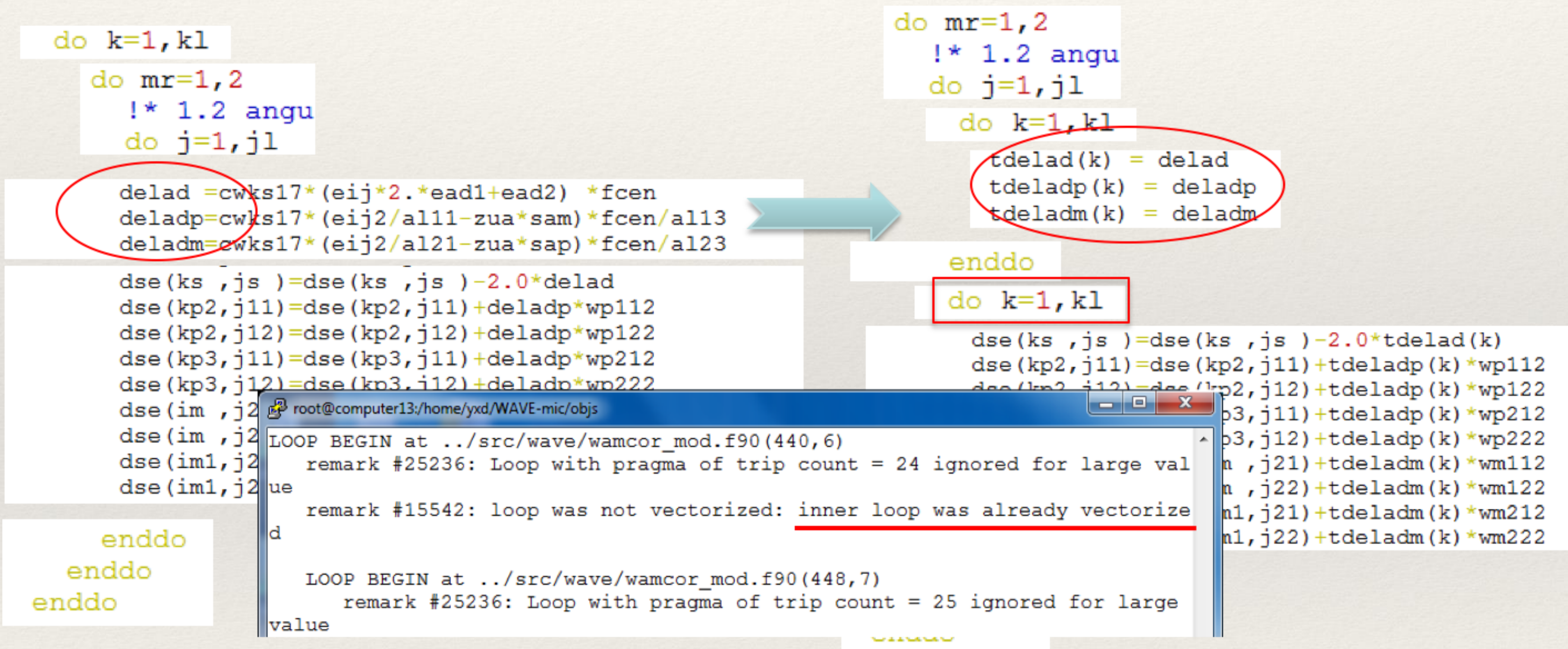
Step 2.3: Vectorization Optimization



Exchange the Loop sequence

Optimization strategy

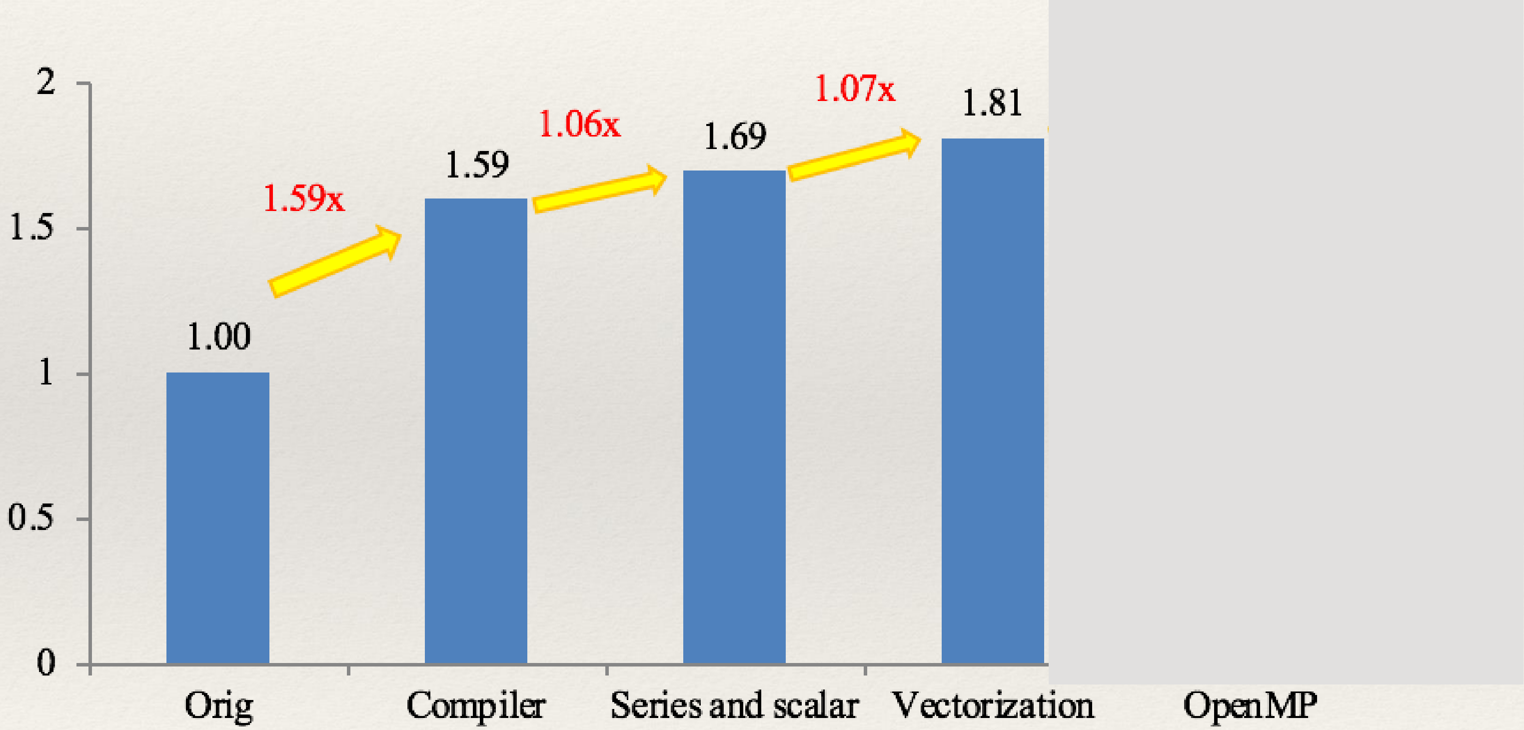
Step 2.3: Vectorization Optimization



Remove the dependence

Optimization strategy

Step 2.3: Vectorization Optimization



Optimization strategy

Step 2.4: Fine-Grained Parallelism

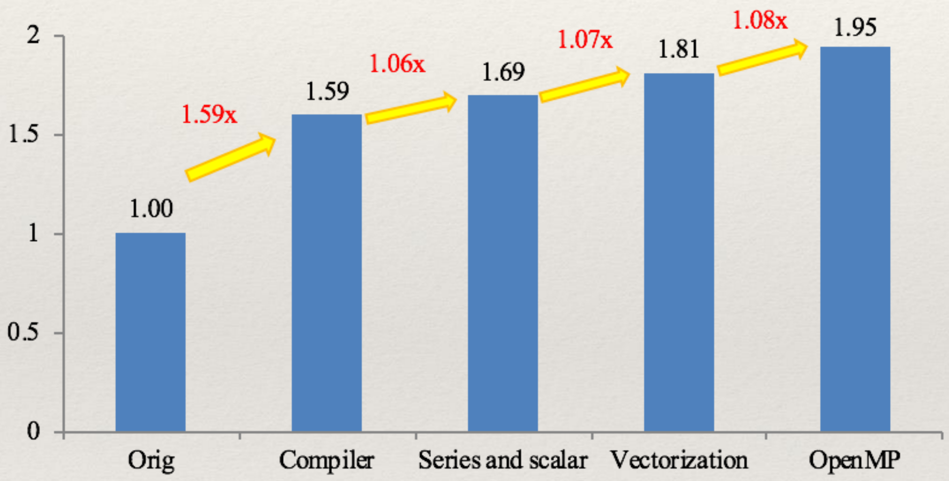
```
!$OMP PARALLELDO PRIVATE(idx)
    do idx=1,np
    call mean2(idx)
    enddo

    allocate(tad(klp1) )
    allocate(tadp(klp1) )
    allocate(tadm(klp1) )
    allocate(tdelad(klp1))
    allocate(tdeladm(klp1))
    allocate(tdeladp(klp1))
    allocate(tkh(klp1))
!$OMP PARALLELDO DEFAULT(NONE) SHARED(pein,peds,pebo,nsp,awk,wx,wy)&
!$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)
&
!$OMP PRIVATE(awkss,vx,vy,ww,wkpm,wkpmt,wakt,beta)&
!$OMP PRIVATE(xx,wp11,wp12,wp21,wp22,wm11,wm12,wm21,wm22)&
!$OMP PRIVATE(wp112,wp122,wp212,wp222,wm112,wm122,wm212,wm222,ffacp,ffacp1)&
!$OMP PRIVATE(cwks17,rij,eij,ea1,ea2,ea3,ea4,ea5,ea6,ea7,ea8,up,up1)&
!$OMP PRIVATE(um,um1,sap,sam,eij2,zua,ead1,ead2,fcen,ad,adp,adm,delad)&
!$OMP PRIVATE(deladm,cd,theta0,costh,sinth,wl,wlstar,wk0,wf0,ws0,bett)&
!$OMP PRIVATE(awfss,arkss,aess,eks,ekspm,sds,asiss,ssds,d0,dk,ssbo,duxdx0)&
!$OMP PRIVATE(duydx0,duydy0,th0,cost2,sint2,cg,cp,cgdc,cu1,cu2,cu3,sscu)&
!$OMP PRIVATE(wstar,deltee,eef,gadiag,eefab,sig,deladp,duxdy0,sbo)&
!$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

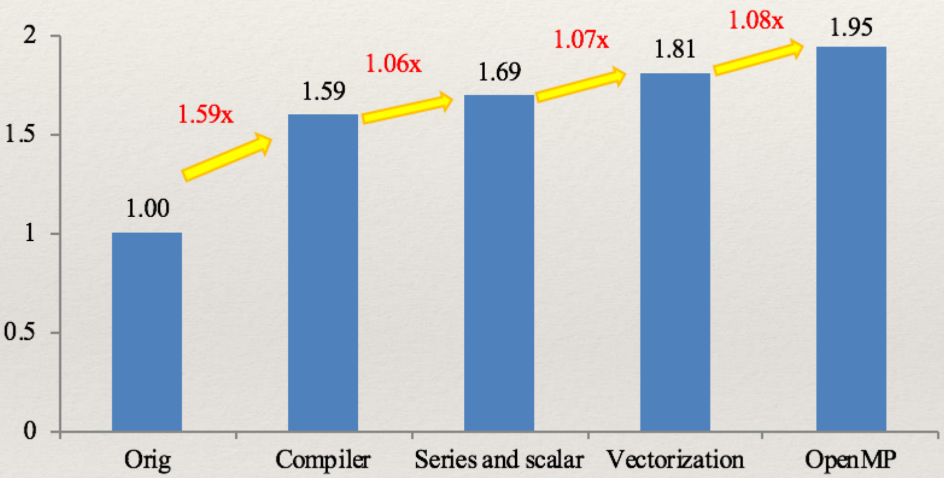
Optimization strategy

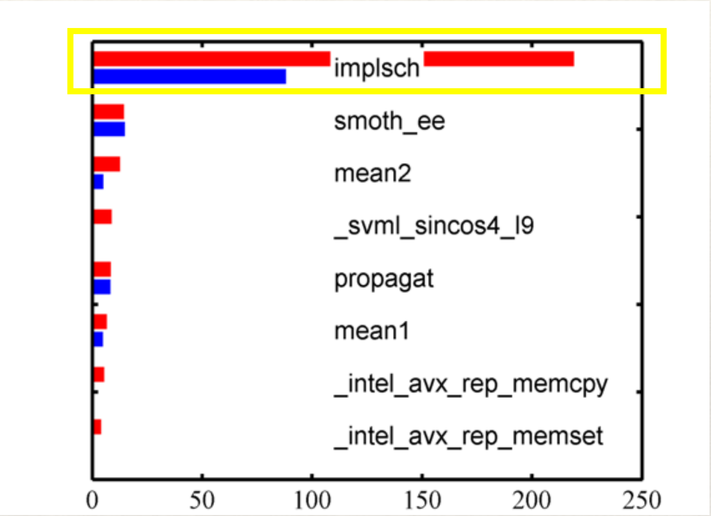
Step 2.4: Fine-Grained Parallism



Optimization strategy

Step 2.4: Fine-Grained Parallism





Time (s)

Optimization strategy

Based on Code Modernization Optimization

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

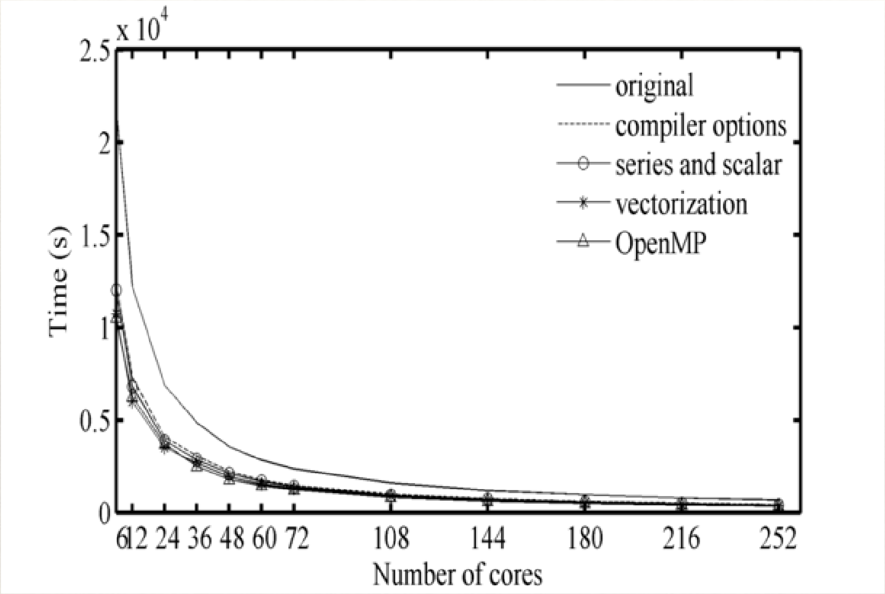
- Optimized on Single Node
  - Scalar optimization
  - Vector optimization
  - Improve Memory access Efficiency
  - Fine-Grained Parallelism

- Optimized on Cluster Level
  - Extend the optimization to multi nodes

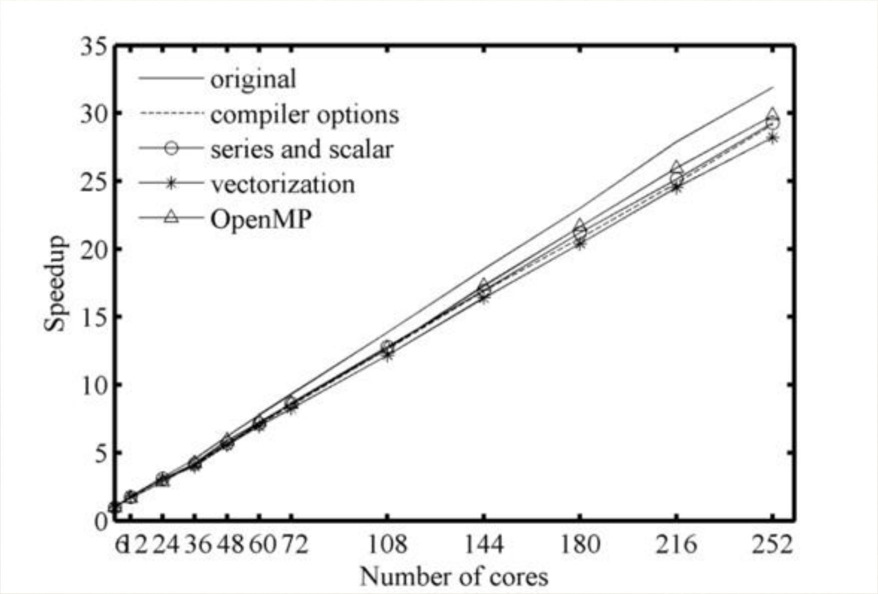
Optimization Methodology

Optimization strategy

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

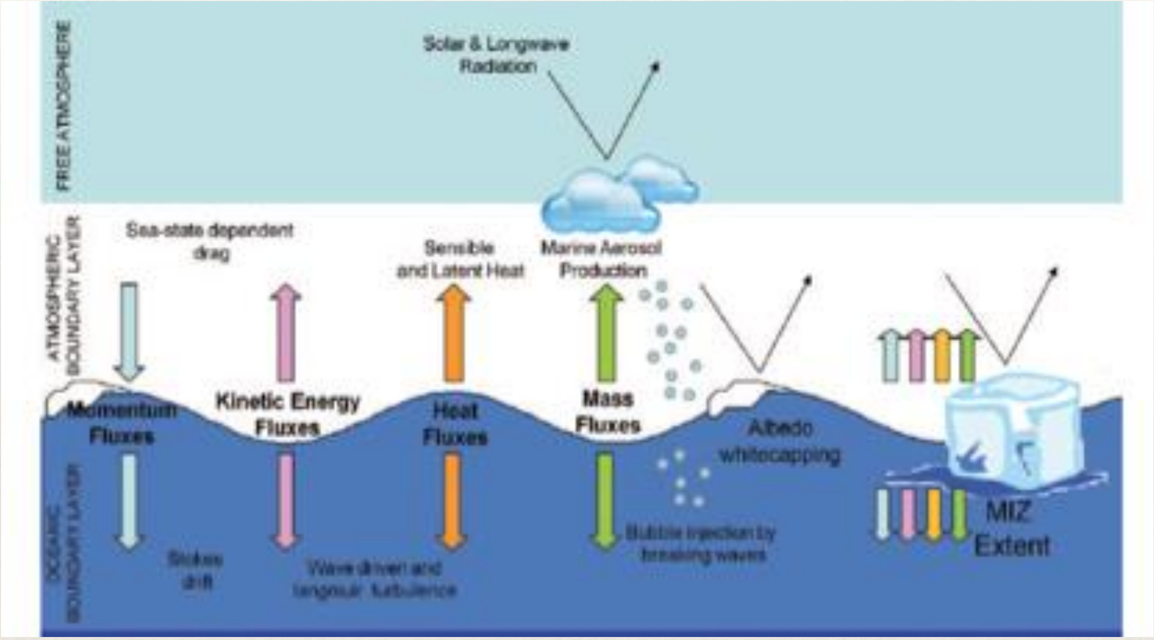
- Optimize on the new Intel Architecture (wider vector length)
- Optimize the MASNUM surface wave model on large-scale cluster
- Try to apply the optimization strategy to other ocean and atmosphere models

THANK FOR YOUR ATTENTION

Contact: songroy@fio.org.cn

Coupled models by incorporated ocean surface wave model

Importance of ocean surface wave

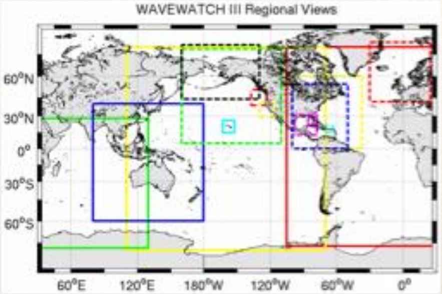


- Ocean surface wave is also important in the ocean and climate system.
- Coupled with ocean surface wave model is a way to accurate simulating and forecasting for ocean and climate

Intel® PCC at FIO

T1: Model computing performance——simulating faster

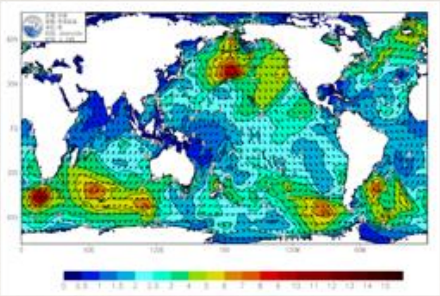
NCEP (USA),
WaveWatch III
Global: 1.25 x 1.00°
Region: 0.25 x 0.25°

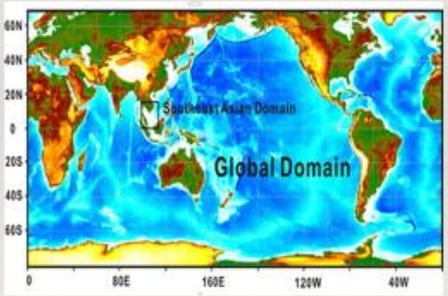


ECMWF (Europe),
WAM, Global
7-day: 0.125 x 0.125°
15-day: 0.25 x 0.25°

State-of-the-art of wave forecasting

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



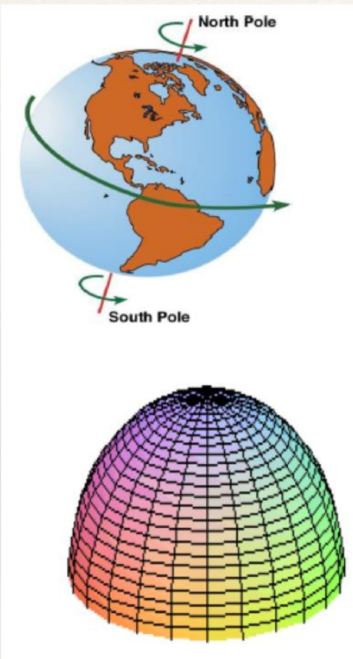


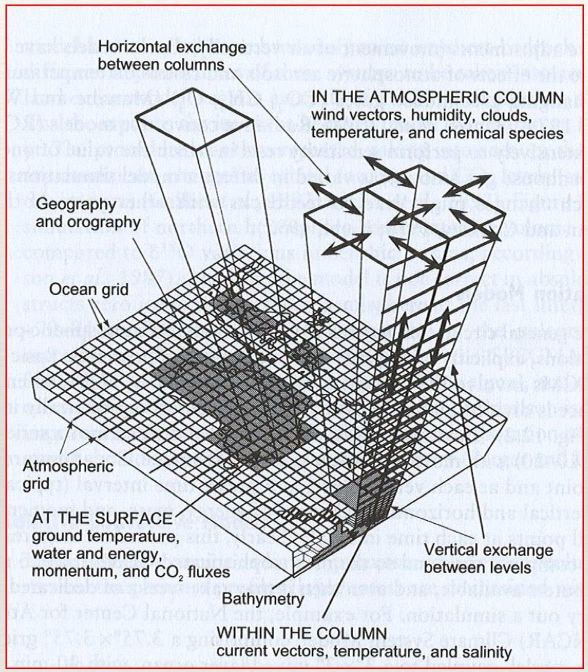
IOC/WESTPAC,
MASNUM
Global: 0.5 x 0.5°
Region: 0.125 x 0.125°

- ✣ 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





Parameterization: unsolved physical process due to resolution

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