Auto-tuning on NUMA and Many-core Environments with an FDM code

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The Twelfth International Workshop on Automatic Performance Tuning
June 2, 2017, Buena Vista Palace Hotel, Orlando, Florida USA
Case-study of auto-tuning and optimization, 14:00 - 14:30
Chair: Toshiyuki Imamura, RIKEN AICS, Japan

Outline

- Background
- An Auto-tuning (AT) Language: *ppOpen-AT* and Adapting AT to an FDM code
- Performance Evaluation with KNL (Knights Landing)
- Conclusion

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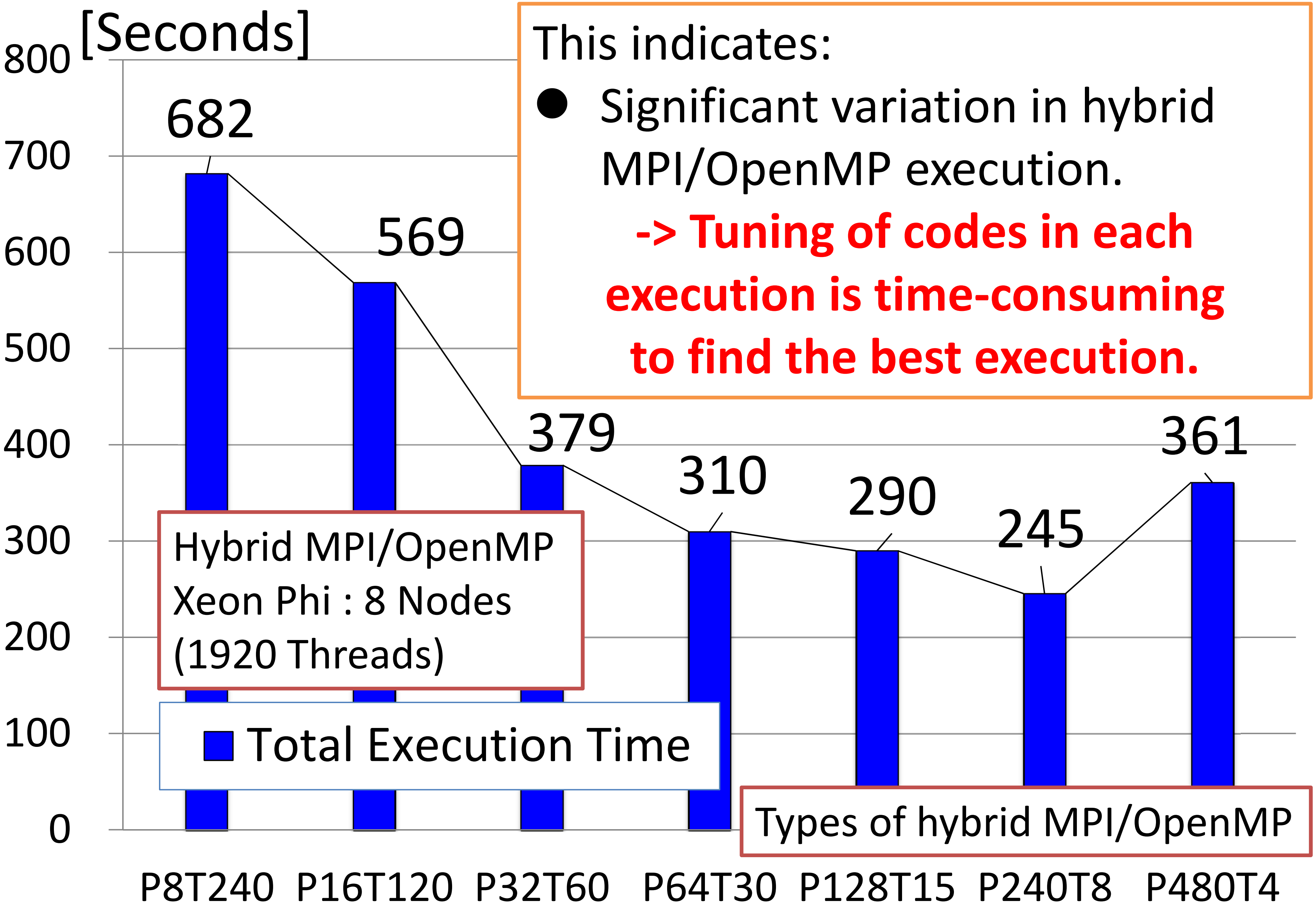
A Motivating Example (An simulation based on FDM)

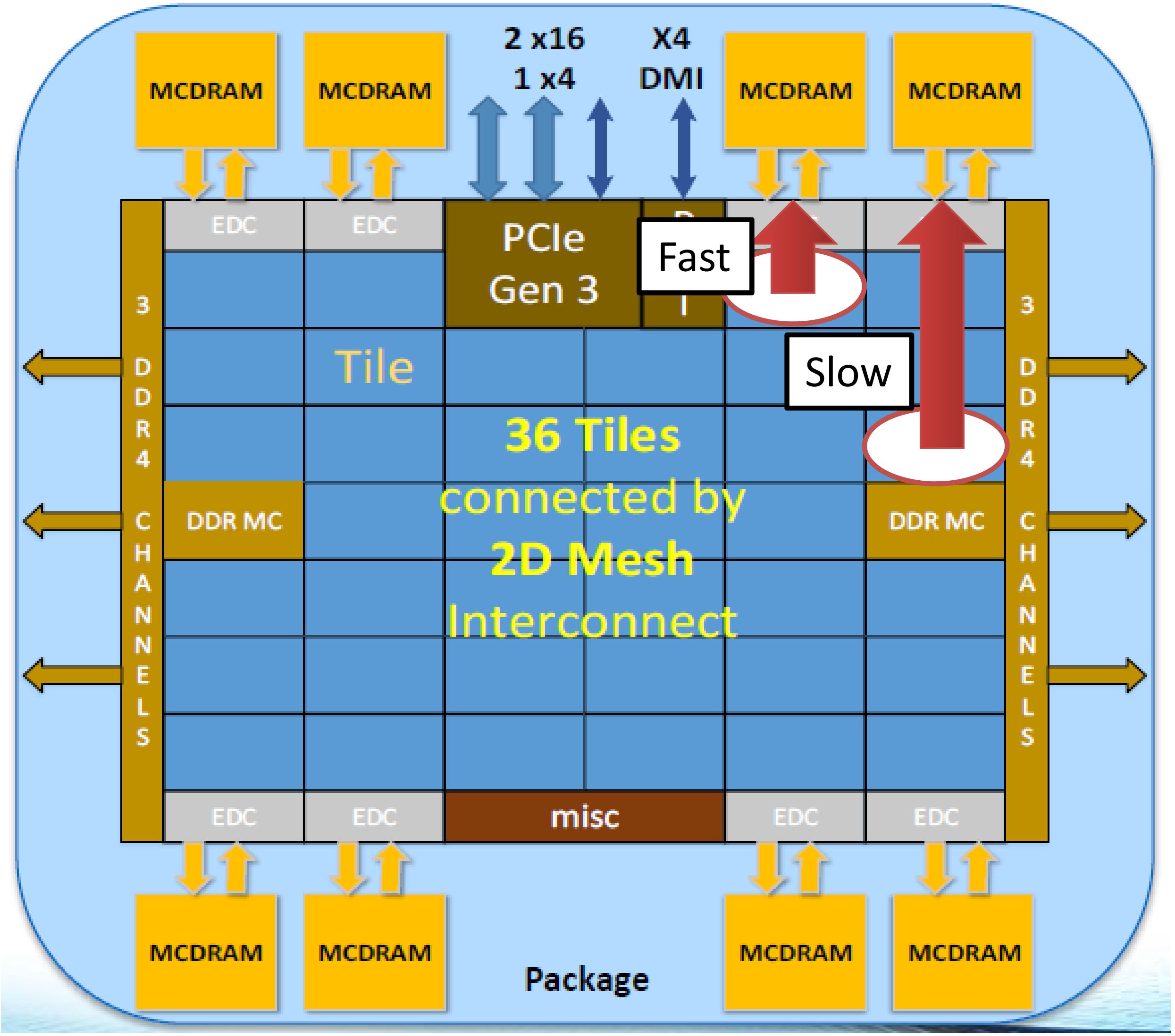


This indicates:

- Significant variation in hybrid MPI/OpenMP execution.

-> Tuning of codes in each execution is time-consuming to find the best execution.

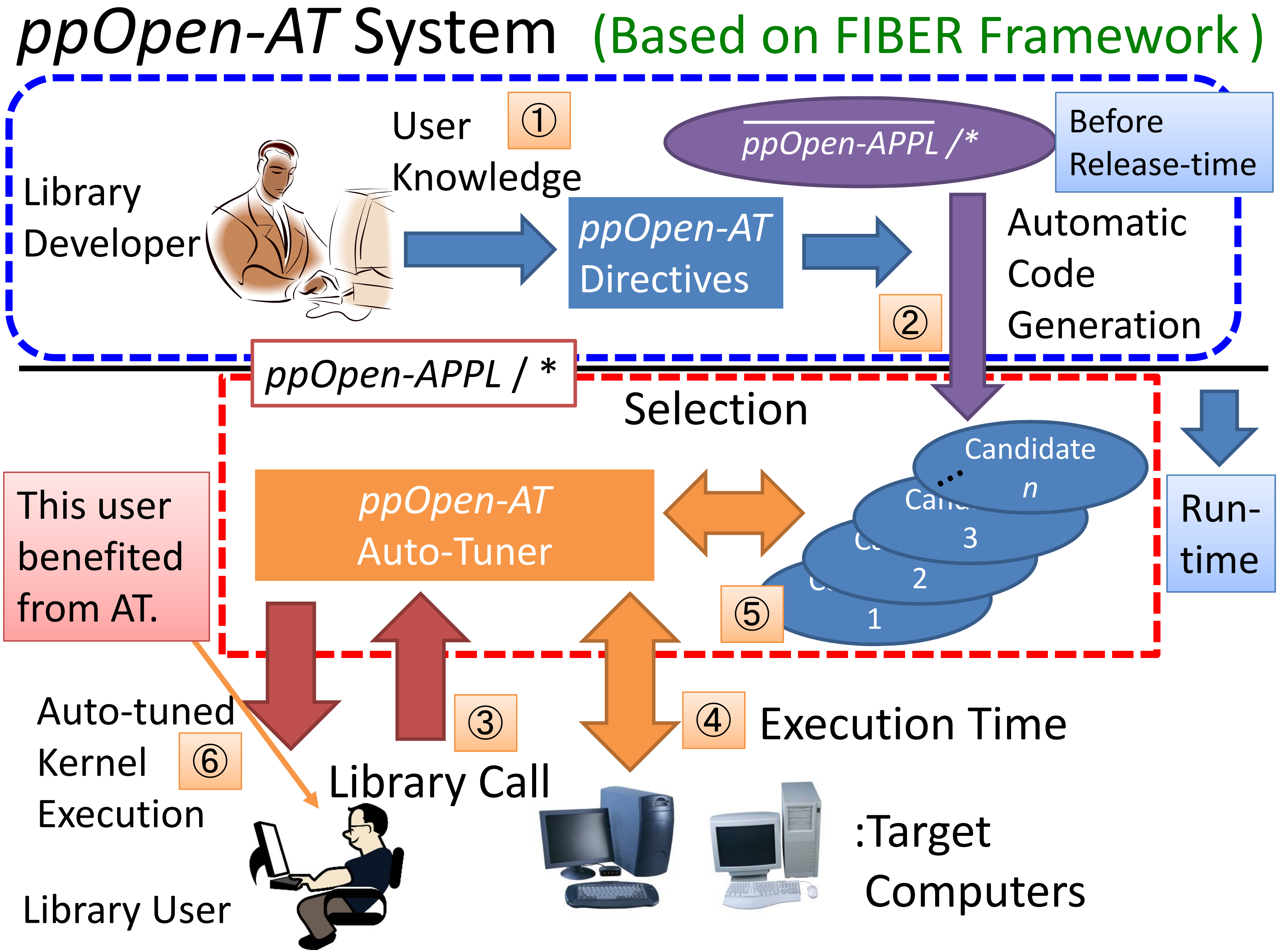
Current Many-core Architectures



Intel Xeon Phi (Knights Landing)

- Many Cores
  68 Physical Cores, Maximum 272 Threads, For each CPU
- Non Uniform Memory Access (NUMA)

Source: Knights Landing (KNL): 2nd Generation Intel® Xeon Phi™ Processor, Avinash Sodani KNL Chief Architect Senior Principal Engineer, Intel Corp.


ppOpen-AT System (Based on FIBER Framework)
Library Developer
User Knowledge
①
ppOpen-APPL /*
Before Release-time
ppOpen-AT Directives
②
Automatic Code Generation
ppOpen-APPL / *
Selection
Candidate n
3
2
1
ppOpen-AT Auto-Tuner
⑤
Run-time
This user benefited from AT.
Auto-tuned Kernel Execution
⑥
③
Library Call
④
Execution Time
:Target Computers
Library User

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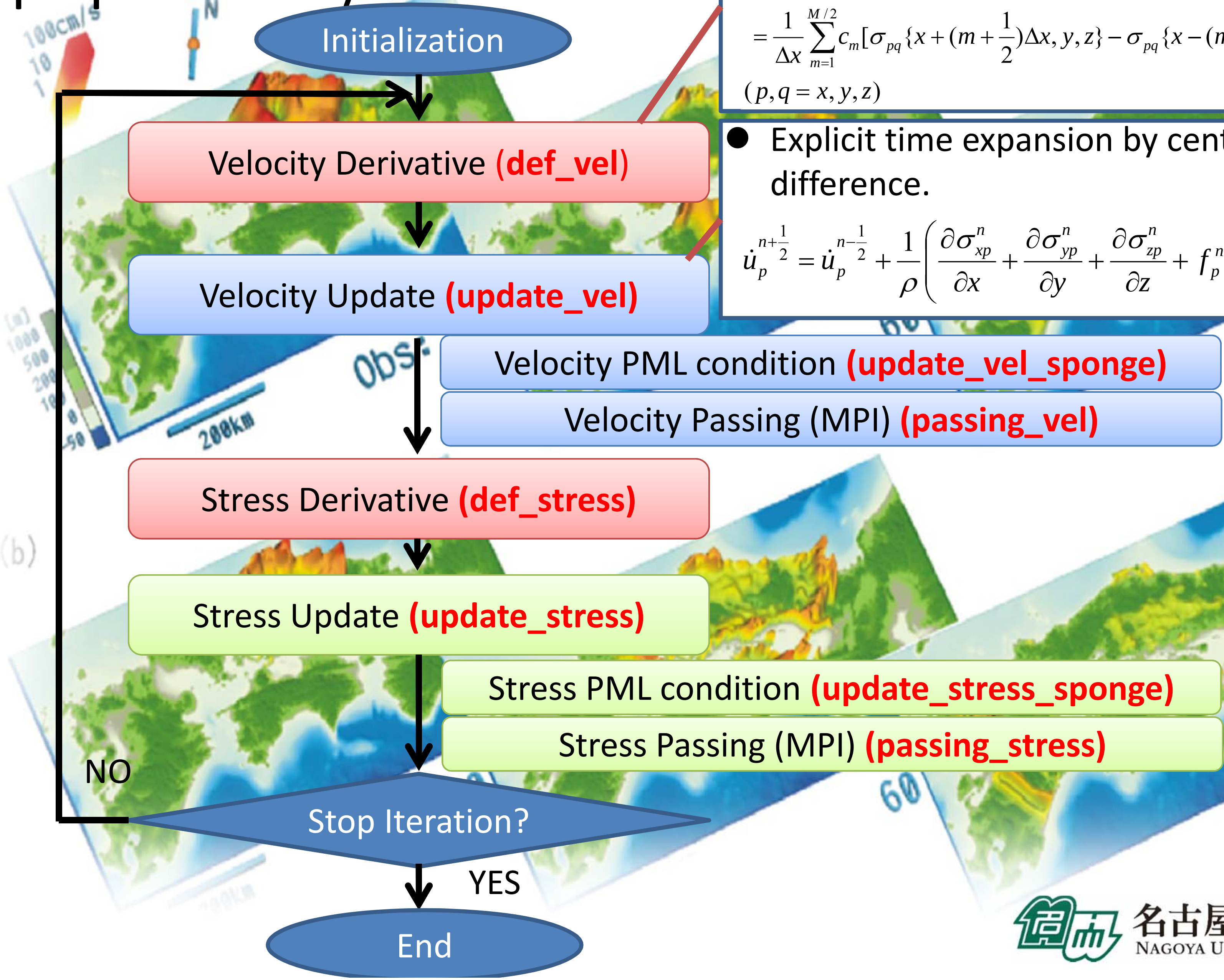
Target Application

- **Seism3D**:
  Simulation for seismic wave analysis.
- Developed by Professor T. Furumura
  at the University of Tokyo.
  – The code is re-constructed as ppOpen-APPL/FDM.
- Finite Differential Method (FDM)
- 3D simulation
  – 3D arrays are allocated.
- Data type: Single Precision (real*4)

Flow Diagram of ppOpen-APPL/FDM



- Space difference by FDM.

$$\frac{d}{dx}\sigma_{pq}(x,y,z)$$

$$=\frac{1}{\Delta x}\sum_{m=1}^{M/2} c_m\left[\sigma_{pq}\{x+(m+\frac{1}{2})\Delta x,y,z\}-\sigma_{pq}\{x-(m-\frac{1}{2})\Delta x,y,z\}\right],$$

$$(p,q=x,y,z)$$

- Explicit time expansion by central difference.

$$\dot{u}_p^{n+\frac{1}{2}}=\dot{u}_p^{n-\frac{1}{2}}+\frac{1}{\rho}\left(\frac{\partial\sigma_{xp}^n}{\partial x}+\frac{\partial\sigma_{yp}^n}{\partial y}+\frac{\partial\sigma_{zp}^n}{\partial z}+f_p^n\right)\Delta t,(p=x,y,z)$$

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AT WITH LOOP TRANSFORMATION

Original Code

A Flow Dependency

```
DO K = 1, NZ
DO J = 1, NY
DO I = 1, NX
  RL  = LAM (I,J,K)
  RM  = RIG (I,J,K)
  RM2 = RM + RM
  RLTHETA = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
  QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
  SXX (I,J,K) = ( SXX (I,J,K)+ (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
  SYY (I,J,K) = ( SYY (I,J,K)+ (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
  SZZ (I,J,K) = ( SZZ (I,J,K) + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
  RMAXY = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K) + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
  RMAXZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K) + 1.0/RIG(I,J,K+1) + 1.0/RIG(I+1,J,K+1))
  RMAYZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I,J+1,K)  + 1.0/RIG(I,J,K+1) + 1.0/RIG(I,J+1,K+1))
  SXY (I,J,K) = ( SXY (I,J,K)   + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT) * QG
  SXZ (I,J,K) = ( SXZ (I,J,K)   + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT) * QG
  SYZ (I,J,K) = ( SYZ (I,J,K)    + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT) * QG
END DO
END DO
END DO
```

Loop Collapse – One dimensional

Merit: Loop length is huge.
This is good for OpenMP thread parallelism.

```
DO KK = 1, NZ * NY * NX
   K = (KK-1)/(NY*NX) + 1
   J = mod((KK-1)/NX,NY) + 1
   I = mod(KK-1,NX) + 1
   RL  = LAM (I,J,K)
   RM  = RIG (I,J,K)
   RM2 = RM + RM
   RMAXY = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K)  + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
   RMAXZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K)  + 1.0/RIG(I,J,K+1) + 1.0/RIG(I+1,J,K+1))
   RMAYZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I,J+1,K)  + 1.0/RIG(I,J,K+1) + 1.0/RIG(I,J+1,K+1))
   RLTHETA = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
   QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
   SXX (I,J,K) = ( SXX (I,J,K)  + (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
   SYY (I,J,K) = ( SYY (I,J,K)  + (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
   SZZ (I,J,K) = ( SZZ (I,J,K)  + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
   SXY (I,J,K) = ( SXY (I,J,K)  + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT )*QG
   SXZ (I,J,K) = ( SXZ (I,J,K)  + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT )*QG
   SYZ (I,J,K) = ( SYZ (I,J,K)  + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT )*QG
END DO
```

Loop Collapse – Two dimensional

Merit: Loop length is huge.
This is good for OpenMP thread parallelism.

This I-loop enables us an opportunity of pre-fetching

```
DO KK = 1, NZ * NY
  K = (KK-1)/NY +  1
  J = mod(KK-1,NY) + 1
  DO I = 1, NX
    RL  = LAM (I,J,K)
    RM  = RIG (I,J,K)
    RM2 = RM + RM
    RMAXY = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K)  + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
    RMAXZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I+1,J,K)  + 1.0/RIG(I,J,K+1) + 1.0/RIG(I+1,J,K+1))
    RMAYZ = 4.0/(1.0/RIG(I,J,K) + 1.0/RIG(I,J+1,K)  + 1.0/RIG(I,J,K+1) + 1.0/RIG(I,J+1,K+1))
    RLTHETA = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
    QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
    SXX (I,J,K) = ( SXX (I,J,K)  + (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
    SYY (I,J,K) = ( SYY (I,J,K)  + (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
    SZZ (I,J,K) = ( SZZ (I,J,K)  + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
    SXY (I,J,K) = ( SXY (I,J,K)  + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT )*QG
    SXZ (I,J,K) = ( SXZ (I,J,K)  + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT )*QG
    SYZ (I,J,K) = ( SYZ (I,J,K)  + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT )*QG
  ENDDO
END DO
```

Loop Split with Re-Computation

```
DO K = 1, NZ
DO J = 1, NY
DO I = 1, NX
   RL  = LAM (I,J,K)
   RM  = RIG (I,J,K)
   RM2 = RM + RM
   RLTHETA  = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
   QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
   SXX (I,J,K) = ( SXX (I,J,K)  + (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
   SYY (I,J,K) = ( SYY (I,J,K)  + (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
   SZZ (I,J,K) = ( SZZ (I,J,K)   + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
ENDDO
DO I = 1, NX
   STMP1 = 1.0/RIG(I,J,K)
   STMP2 = 1.0/RIG(I+1,J,K)
   STMP4 = 1.0/RIG(I,J,K+1)
   STMP3 = STMP1 + STMP2
   RMAXY = 4.0/(STMP3  + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
   RMAXZ = 4.0/(STMP3  + STMP4 + 1.0/RIG(I+1,J,K+1))
   RMAYZ = 4.0/(STMP3  + STMP4 + 1.0/RIG(I,J+1,K+1))
   QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
   SXY (I,J,K) = ( SXY (I,J,K) + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT )*QG
   SXZ (I,J,K) = ( SXZ (I,J,K) + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT )*QG
   SYZ (I,J,K) = ( SYZ (I,J,K)  + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT )*QG
END DO
END DO
END DO
```

Re-computation is needed.
⇒Compilers do not apply it without directive.

Perfect Splitting

```
DO K = 1, NZ
DO J = 1, NY
DO I = 1, NX
   RL  = LAM (I,J,K)
   RM  = RIG (I,J,K)
   RM2 = RM + RM
   RLTHETA  = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
   QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
   SXX (I,J,K) = ( SXX (I,J,K)  + (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
   SYY (I,J,K) = ( SYY (I,J,K)  + (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
   SZZ (I,J,K) = ( SZZ (I,J,K)   + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
ENDDO;  ENDDO; ENDDO
```

Perfect Splitting

```
DO K = 1, NZ
DO J = 1, NY
DO I = 1, NX
   STMP1 = 1.0/RIG(I,J,K)
   STMP2 = 1.0/RIG(I+1,J,K)
   STMP4 = 1.0/RIG(I,J,K+1)
   STMP3 = STMP1 + STMP2
   RMAXY = 4.0/(STMP3  + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
   RMAXZ = 4.0/(STMP3  + STMP4 + 1.0/RIG(I+1,J,K+1))
   RMAYZ = 4.0/(STMP3  + STMP4 + 1.0/RIG(I,J+1,K+1))
   QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
   SXY (I,J,K) = ( SXY (I,J,K) + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT )*QG
   SXZ (I,J,K) = ( SXZ (I,J,K) + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT )*QG
   SYZ (I,J,K) = ( SYZ (I,J,K)  + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT )*QG
END DO;  END DO;  END DO;
```

ppOpen-AT Directives

: Loop Split & Collapse with data-flow dependence

```
!oat$ install LoopFusionSplit region start
!$omp parallel do private(k,j,i,STMP1,STMP2,STMP3,STMP4,RL,RM,RM2,RMAXY,RMAXZ,RMAYZ,RLTHETA,QG)
    DO K = 1, NZ
    DO J = 1, NY
    DO I = 1, NX
       RL  = LAM (I,J,K);   RM  = RIG (I,J,K);   RM2 = RM + RM
       RLTHETA  = (DXVX(I,J,K)+DYVY(I,J,K)+DZVZ(I,J,K))*RL
!oat$ SplitPointCopyDef  region  start
       QG  = ABSX(I)*ABSY(J)*ABSZ(K)*Q(I,J,K)
!oat$ SplitPointCopyDef  region  end
       SXX (I,J,K) = ( SXX (I,J,K) + (RLTHETA + RM2*DXVX(I,J,K))*DT )*QG
       SYY (I,J,K) = ( SYY (I,J,K) + (RLTHETA + RM2*DYVY(I,J,K))*DT )*QG
       SZZ (I,J,K) = ( SZZ (I,J,K) + (RLTHETA + RM2*DZVZ(I,J,K))*DT )*QG
!oat$ SplitPoint  (K, J, I)
       STMP1 = 1.0/RIG(I,J,K);  STMP2 = 1.0/RIG(I+1,J,K);  STMP4 = 1.0/RIG(I,J,K+1)
       STMP3 = STMP1 + STMP2
       RMAXY = 4.0/(STMP3 + 1.0/RIG(I,J+1,K) + 1.0/RIG(I+1,J+1,K))
       RMAXZ = 4.0/(STMP3 + STMP4 + 1.0/RIG(I+1,J,K+1))
       RMAYZ = 4.0/(STMP3 + STMP4 + 1.0/RIG(I,J+1,K+1))
!oat$ SplitPointCopyInsert
       SXY (I,J,K) = ( SXY (I,J,K) + (RMAXY*(DXVY(I,J,K)+DYVX(I,J,K)))*DT )*QG
       SXZ (I,J,K) = ( SXZ (I,J,K) + (RMAXZ*(DXVZ(I,J,K)+DZVX(I,J,K)))*DT )*QG
       SYZ (I,J,K) = ( SYZ (I,J,K) + (RMAYZ*(DYVZ(I,J,K)+DZVY(I,J,K)))*DT )*QG
    END DO;  END DO;  END DO
!$omp end parallel do
!oat$ install LoopFusionSplit region end
```

Specify Loop Split and Loop Fusion

Re-calculation is defined.

Loop Split Point

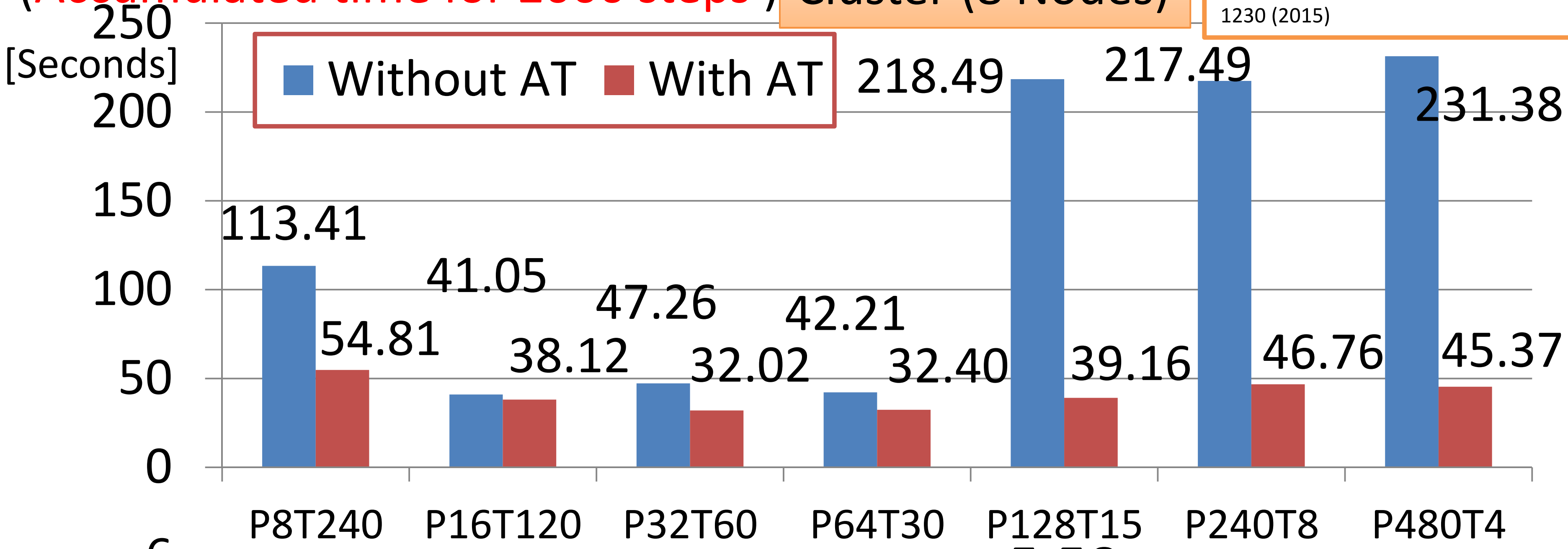
Using the re-calculation is defined.

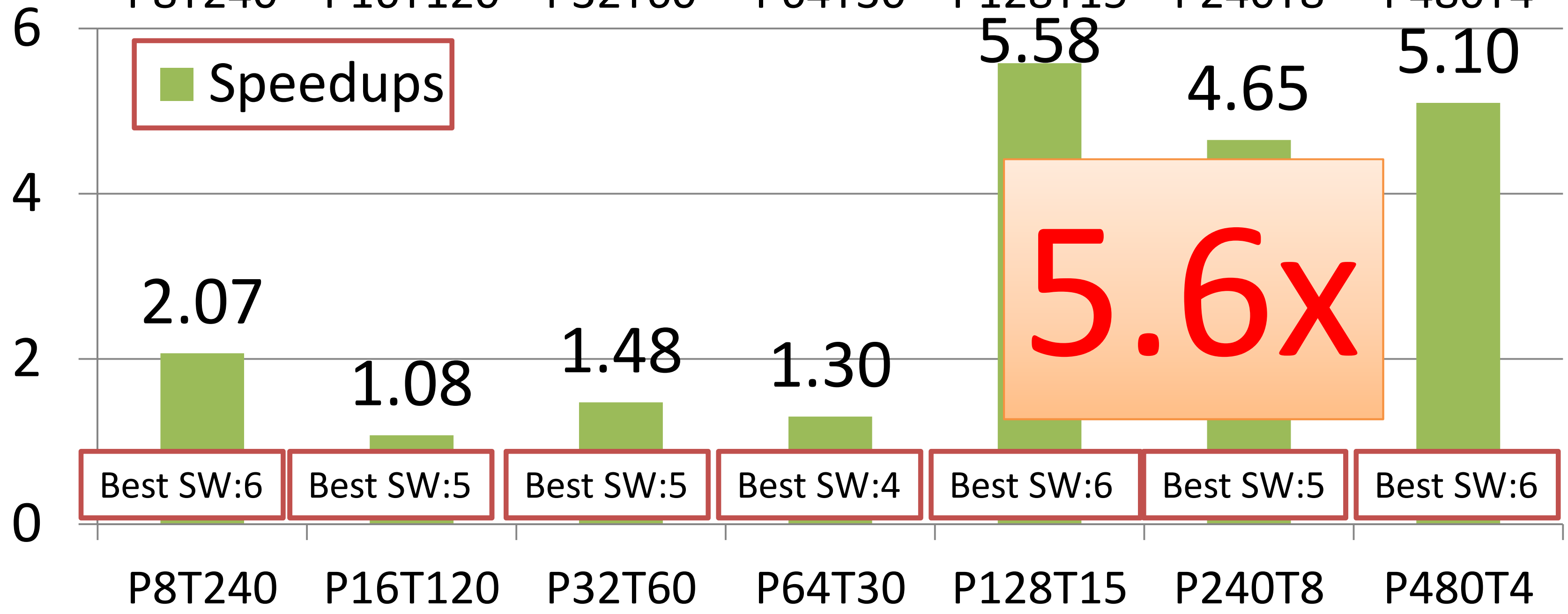
AT Effect (update_stress)

(Accumulated time for 2000 steps)

Xeon Phi (KNC) Cluster (8 Nodes)

T. Katagiri, S. Ohshima, M. Matsumoto: "Directive-based Auto-tuning for the Finite Difference Method on the Xeon Phi", Proc. of IPDPSW2015, pp.1221-1230 (2015)





AT WITH CODE SELECTION

Original Implementation (For Vector Machines)

Fourth-order accurate central-difference scheme for velocity. (**def_stress**)

```
call ppohFDM_pdiffx3_m4_OAT( VX,DXVX, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
call ppohFDM_pdiffy3_p4_OAT( VX,DYVX, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
call ppohFDM_pdiffz3_p4_OAT( VX,DZVX, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
call ppohFDM_pdiffy3_m4_OAT( VY,DYVY, NXP,NYP,NZP,NXP0,NXP1,NYP0,… )
call ppohFDM_pdiffx3_p4_OAT( VY,DXVY, NXP,NYP,NZP,NXP0,NXP1,NYP0,… )
call ppohFDM_pdiffz3_p4_OAT( VY,DZVY, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
call ppohFDM_pdiffx3_p4_OAT( VZ,DXVZ, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
call ppohFDM_pdiffy3_p4_OAT( VZ,DYVZ, NXP,NYP,NZP,NXP0,NXP1,NYP0,… )
call ppohFDM_pdiffz3_m4_OAT( VZ,DZVZ, NXP,NYP,NZP,NXP0,NXP1,NYP0,…)
```

```
 if( is_fs .or. is_nearfs ) then
       call ppohFDM_bc_vel_deriv( KFSZ,NIFS,NJFS,IFSX,IFSY,IFSZ,JFSX,JFSY,JFSZ )
end if
```

Process of model boundary.

```
call ppohFDM_update_stress(1, NXP, 1, NYP, 1, NZP)
```

Explicit time expansion by leap-frog scheme. (update_stress)

Original Implementation (For Vector Machines)

```
subroutine OAT_InstallppohFDMupdate_stress(..)
!$omp parallel do private(i,j,k,RL1,RM1,RM2,RLRM2,DXVX1,DYVY1,DZVZ1,…)
  do k = NZ00, NZ01
    do j = NY00, NY01
      do i = NX00, NX01
        RL1   = LAM (I,J,K); RM1   = RIG (I,J,K);  RM2   = RM1 + RM1; RLRM2 = RL1+RM2
        DXVX1 = DXVX(I,J,K);  DYVY1 = DYVY(I,J,K);  DZVZ1 = DZVZ(I,J,K)
        D3V3  = DXVX1 + DYVY1 + DZVZ1
        SXX (I,J,K) = SXX (I,J,K) + (RLRM2*(D3V3)-RM2*(DZVZ1+DYVY1) ) * DT
        SYY (I,J,K) = SYY (I,J,K)  + (RLRM2*(D3V3)-RM2*(DXVX1+DZVZ1) ) * DT
        SZZ (I,J,K) = SZZ (I,J,K)  + (RLRM2*(D3V3)-RM2*(DXVX1+DYVY1) ) * DT
        DXVYDYVX1 = DXVY(I,J,K)+DYVX(I,J,K);  DXVZDZVX1 = DXVZ(I,J,K)+DZVX(I,J,K)
        DYVZDZVY1 = DYVZ(I,J,K)+DZVY(I,J,K)
        SXY (I,J,K) = SXY (I,J,K) + RM1 * DXVYDYVX1 * DT
        SXZ (I,J,K) = SXZ (I,J,K) + RM1 * DXVZDZVX1 * DT
        SYZ (I,J,K) = SYZ (I,J,K) + RM1 * DYVZDZVY1 * DT
      end do
    end do
  end do
retuen
end
```

Explicit time expansion by leap-frog scheme. (update_stress)

Input and output for arrays in each call -> Increase of B/F ratio: ~1.7

The Code Variants (For Scalar Machines)

- Variant1 (IF-statements inside)
  - The followings include inside loop:
  1. Fourth-order accurate central-difference scheme for velocity.
  2. Process of model boundary.
  3. Explicit time expansion by leap-frog scheme.
- Variant2 (IF-free, but there is IF-statements inside loop for process of model boundary.)
  - To remove IF sentences from the variant1, the loops are reconstructed.
  - The order of computations is changed, but the result without round-off errors is same.
  - **[Main Loop]**
  1. Fourth-order accurate central-difference scheme for velocity.
  2. Explicit time expansion by leap-frog scheme.
  - **[Loop for process of model boundary]**
  1. Fourth-order accurate central-difference scheme for velocity.
  2. Process of model boundary.
  3. Explicit time expansion by leap-frog scheme.

Variant1 (For Scalar Machines)

Stress tensor of Sxx, Syy, Szz

```
 !$omp parallel do   private
(i,j,k,RL1,RM1,RM2,RLRM2,DXVX, …)
 do k_j=1, (NZ01-NZ00+1)*(NY01-NY00+1)
   k=(k_j-
   j=mod(
   do i = N
      RL1
      RM2
  !4th ord
     DXV
        - (VX(I+1,J,K)-VX(I-2,J,K))*C41/dx
     DYVY0 = (VY(I,J,K)  -VY(I,J-1,K))*C40/dy &
        - (VY(I,J+1,K)-VY(I,J-2,K))*C41/dy
     DZVZ0 = (VZ(I,J,K)  -VZ(I,J,K-1))*C40/dz &
        - (VZ(I,J,K+1)-VZ(I,J,K-2))*C41/dz
! truncate_diff_vel
! X dir
      if (idx==0) then
        if (i==1)then
          DXVX0 = ( VX(1,J,K) - 0.0_PN    )/ DX
        end if
        if (i==2) then
          DXVX0 = ( VX(2,J,K) - VX(1,J,K) )/ DX
         end if
      end if
      if( idx == IP-1 ) then
        if (i==NXP)then
    DXVX0 = ( VX(NXP,J,K) - VX(NXP-1,J,K) ) /  DX
        end if
```

Fourth-order accurate central-difference scheme for velocity.

```
! Y dir
      if( idy == 0 ) then ! Shallowmost
        if (j==1)then
          DYVY0 = ( VY(I,1,K) - 0.0_
        end if
        if (j==2)then
          DYVY0 = ( VY(I,2,K) - VY(
        end if
      end if
      if( idy == JP-1 ) then
        if (j==NYP)then
          DYVY0 = ( VY(I,NYP,K) - V
        end if
      end if
! Z dir
      if( idz == 0 ) then ! Shallowmost
        if (k==1)then
          DZVZ0 = ( VZ(I,J,1) - 0.0_
        end if
        if (k==2)then
          DZVZ0 = ( VZ(I,J,2) - VZ(
        end if
      end if
      if( idz == KP-1 ) then
        if (k==NZP)then
          DZVZ0 = ( VZ(I,J,NZP) -
        end if
      end if
```

Explicit time expansion by leap-frog scheme

```
DXVX1 = DXVX0;  DYVY1 = DYVY0
DZVZ1 = DZVZ0;  D3V3  = DXVX1 + DYVY1 + DZVZ1
  SXX (I,J,K) = SXX (I,J,K) &
    + (RLRM2*(D3V3)-RM2*(DZVZ1+DYVY1) ) * DT
  SYY (I,J,K) = SYY (I,J,K) &
    + (RLRM2*(D3V3)-RM2*(DXVX1+DZVZ1) ) * DT
  SZZ (I,J,K) = SZZ (I,J,K) &
    + (RLRM2*(D3V3)-RM2*(DXVX1+DYVY1) ) * DT
   end do
 end do
!$omp end parallel do
```

☺B/F ratio is reduced to <u>0.4</u>

☹IF sentences inside – it is difficult to optimize code by compiler.

Process of model boundary.

Variant2 (IF-free)

Stress tensor of Sxx, Syy, Szz

```
!$omp parallel do   private(i,j,k,RL1,RM1,・・・)
do k_j=1, (NZ01-NZ00+1)*(NY01-NY00+1)
  k=(k_j-1)/(NY01-NY00+1)+NZ00
  j=mod((k_j-1),(NY01-NY00+1))+NY00
        = NX00, NX01
           = LAM (I,J,K); RM1   = RIG (I,J,K);
         2   = RM1 + RM1; RLRM2 = RL1+RM2
          rder diff (DXVX,DYVY,DZVZ)
          VX0 = (VX(I,J,K)  -VX(I-1,J,K))*C40/dx -  (VX(I+1,J,K)-VX(I-2,J,K))*C41/dx
          VY0 = (VY(I,J,K)  -VY(I,J-1,K))*C40/dy  - (VY(I,J+1,K)-VY(I,J-2,K))*C41/dy
      DZVZ0 = (VZ(I,J,K)  -VZ(I,J,K-1))*C40/dz  - (VZ(I,J,K+1)-VZ(I,J,K-2))*C41/dz
      DXVX1 = DXVX0; DYVY1 = DYVY0;
      DZVZ1 = DZVZ0;
      D3V3  = DXVX1 + DYVY1 + DZVZ1;
      SXX (I,J,K) = SXX (I,J,K) + (RLRM2*(D3V3)-RM2* (DZVZ1+DYVY1) ) * DT
      SYY (I,J,K) = SYY (I,J,K) + (RLRM2*(D3V3)-RM2* (DXVX1+DZVZ1) ) * DT
      SZZ (I,J,K) = SZZ (I,J,K)  + (RLRM2*(D3V3)-RM2* (DXVX1+DYVY1) ) * DT
    end do
end do
!$omp end parallel do
```

Fourth-order accurate central-difference scheme for velocity.

Explicit time expansion by leap-frog scheme.

☺Win-win between B/F ratio and optimization by compiler.

Variant2 (IF-free)

Loop for process of model boundary

```
! 2nd replace
if( is_fs .or. is_nearfs ) then
!$omp parallel do private(i,j,k,RL1,RM
do i=NX00,NX01
   do j=NY00,NY01
      do k = KFSZ(i,j)-1, KFSZ(i,j)+1, 2
         RL1   = LAM (I,J,K); RM1   = RIG
         RM2   = RM1 + RM1; RLRM2 = RL1+RM2
! 4th order diff
         DXVX0 = (VX(I,J,K)  -VX(I-1,J,K))*C40/dx &
              - (VX(I+1,J,K)-VX(I-2,J,K))*C41/dx
         DYVX0 = (VX(I,J+1,K)-VX(I,J,K)  )*C40/dy &
              - (VX(I,J+2,K)-VX(I,J-1,K))*C41/dy
         DXVY0 = (VY(I+1,J,K)-VY(I  ,J,K))*C40/dx &
             - (VY(I+2,J,K)-VY(I-1,J,K))*C41/dx
         DYVY0 = (VY(I,J,K)  -VY(I,J-1,K))*C40/dy &
             - (VY(I,J+1,K)-VY(I,J-2,K))*C41/dy
         DXVZ0 = (VZ(I+1,J,K)-VZ(I  ,J,K))*C40/dx &
             - (VZ(I+2,J,K)-VZ(I-1,J,K))*C41/dx
         DYVZ0 = (VZ(I,J+1,K)-VZ(I,J,K)  )*C40/dy &
             - (VZ(I,J+2,K)-VZ(I,J-1,K))*C41/dy
         DZVZ0 = (VZ(I,J,K)  -VZ(I,J,K-1))*C40/dz &
              - (VZ(I,J,K+1)-VZ(I,J,K-2))*C41/dz
```

Process of model boundary.

Fourth-order accurate central-difference scheme for velocity

```
! vel derive
   if (K==KFSZ(I,J)+1) then
      DZVX0 = ( VX(I,J,KFSZ(I,J)+2)-VX(I,J,KFSZ(I,J)+1) )/ DZ
      DZVY0 = ( VY(I,J,KFSZ(I,J)+2)-VY(I,J,KFSZ(I,J)+1) )/ DZ
   else if (K==KFSZ(I,J)-1) then
      DZVX0 = ( VX(I,J,KFSZ(I,J)  )-VX(I,J,KFSZ(I,J)-1) )/ DZ
      DZVY0 = ( VY(I,J,KFSZ(I,J)  )-VY(I,J,KFSZ(I,J)-1) )/ DZ
   end if
   DXVX1 = DXVX0
   DYVY1 = DYVY0
   DZVZ1 = DZVZ0
   D3V3  = DXVX1 + DYVY1 + DZVZ1
   DXVYDYVX1 = DXVY0+DYVX0
   DXVZDZVX1 = DXVZ0+DZVX0
   DYVZDZVY1 = DYVZ0+DZVY0
   if (K==KFSZ(I,J)+1)then
      KK=2
   else
      KK=1
   end if
   SXX (I,J,K) = SSXX (I,J,KK) &
      + (RLRM2*(D3V3)-RM2*(DZVZ1+DYVY1) ) * DT
   SYY (I,J,K) = SSYY (I,J,KK) &
      + (RLRM2*(D3V3)-RM2*(DXVX1+DZVZ1) ) * DT
   SZZ (I,J,K) = SSZZ (I,J,KK) &
      + (RLRM2*(D3V3)-RM2*(DXVX1+DYVY1) ) * DT
   SXY (I,J,K) = SSXY (I,J,KK) + RM1 * DXVYDYVX1 * DT
   SXZ (I,J,K) = SSXZ (I,J,KK) + RM1 * DXVZDZVX1 * DT
   SYZ (I,J,K) = SSYZ (I,J,KK) + RM1 * DYVZDZVY1 * DT
      end do
   end do
end do
!$omp end parallel do
```

Explicit time expansion by leap-frog scheme.

Code Selection by ppOpen-AT and Hierarchical AT

Upper Code

With Select clause, code selection can be specified.

```
Program main
....
!OAT$ install select region start
!OAT$ name ppohFDMupdate_vel_select
!OAT$ select sub region start
call ppohFDM_pdiffx3_p4( SXX,DXSXX,NXP,NYP,NZP,....)
call ppohFDM_pdiffy3_p4( SYY,DYSYY, NXP,NYP,NZP,.....)
...
if( is_fs .or. is_nearfs ) then
  call ppohFDM_bc_stress_deriv( KFSZ,NIFS,NJFS,II
end if
call ppohFDM_update_vel    ( 1, NXP, 1, NYP, 1, NZ
!OAT$ select sub region end

!OAT$ select sub region start
Call ppohFDM_update_vel_Intel  ( 1, NXP, 1, NYP,
!OAT$ select sub region end

!OAT$ install select region end
```

Lower Code

```
subroutine ppohFDM_pdiffx3_p4(....)
....
!OAT$ install LoopFusion region start
....
```

```
subroutine ppohFDM_update_vel(....)
....
!OAT$ install LoopFusion region start
!OAT$ name ppohFDMupdate_vel
!OAT$ debug (pp)
!$omp parallel do private(i,j,k,ROX,ROY,ROZ)
do k = NZ00, NZ01
  do j = NY00, NY01
    do i = NX00, NX01
   .....
....
```

The Number of AT Candidates (ppOpen-APPL/FDM)

Kernel Names	AT Objects	The Number of Candidates
1. update_stress	・Loop Collapses and Splits ：8 Kinds ・Code Selections : 2 Kinds	**10**
2. update_vel	・Loop Collapses, Splits, and re-ordering of statements: ：6 Kinds ・Code Selections: 2 Kinds	**8**
3. update_stress_sponge	・Loop Collapses：3 Kinds	**3**
4. update_vel_sponge	・Loop Collapses：3 Kinds	**3**
5. ppohFDM_pdiffx3_p4	Kernel Names：def_update、def_vel ・Loop Collapses：3 Kinds	**3**
6. ppohFDM_pdiffx3_m4		**3**
7. ppohFDM_pdiffy3_p4		**3**
8. ppohFDM_pdiffy3_m4		**3**
9. ppohFDM_pdiffz3_p4		**3**
10.ppohFDM_pdiffz3_m4		**3**
11. ppohFDM_ps_pack	Data packing and unpacking ・Loop Collapses： 3 Kinds	**3**
12. ppohFDM_ps_unpack		**3**
13. ppohFDM_pv_pack		**3**
14. ppohFDM_pv_unpack		**3**

- Total：54 Kinds
- Hybrid MPI/OpenMP: 7 Kinds
- 54×7 = 378 Kinds

Outline

- Background
- An Auto-tuning (AT) Language: *ppOpen-AT* and Adapting AT to an FDM code
- Performance Evaluation with KNL (Knights Landing)
- Conclusion

Oakforest-PACS (ITC, U. Tokyo and CCS, Tsukuba U.) :Fujitsu PRIMERGY CX1640 M1

8,208 Nodes (558,144 Cores)

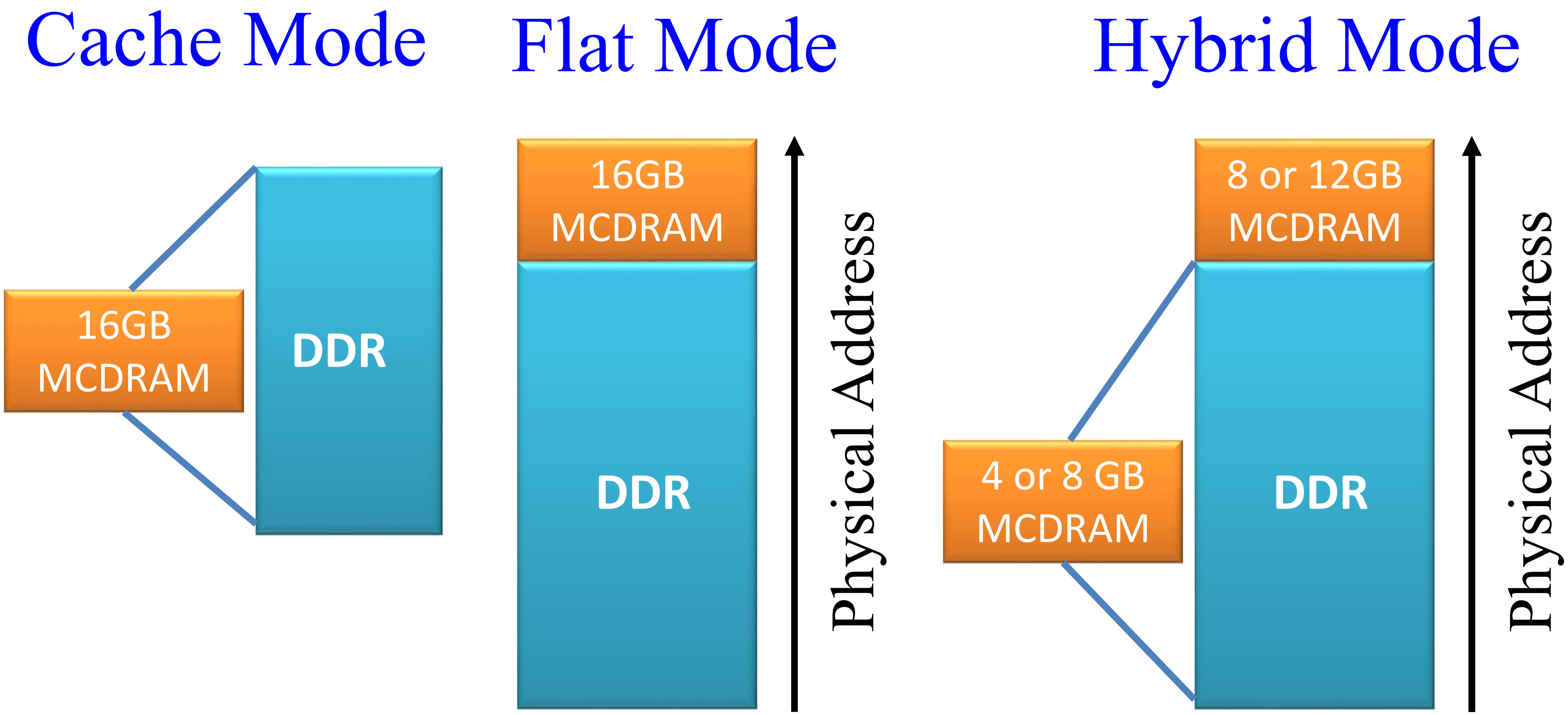
● Total Organization

item	Specification
Total Theoretical Peak	**25.004 PFLOPS**
Total Number of Nodes	8208
Total Memory Amount	897 TByte
Total Storage Amount	26 PB
Total Storage Bandwidth	500 GB/sec
Total Fast Cache Amount	940 TB
Total Fast Cache Bandwidth	1,560 GB/sec

● Node Configuration

CPU	Intel® Xeon Phi ™ 7250 (Knights Landing, KNL)
#Processors	1 (68 Physical Cores)
Frequency	1.4 GHz
Theoretical Peak for each Node	3.0464 Tflops (double) / 6.0928 Tflops (single)
Memory	**96 GB(DDR4)＋ 16 GB(MCDRAM)**
Inter Connect	Intel ® Omni-Path Network (100 Gbps)

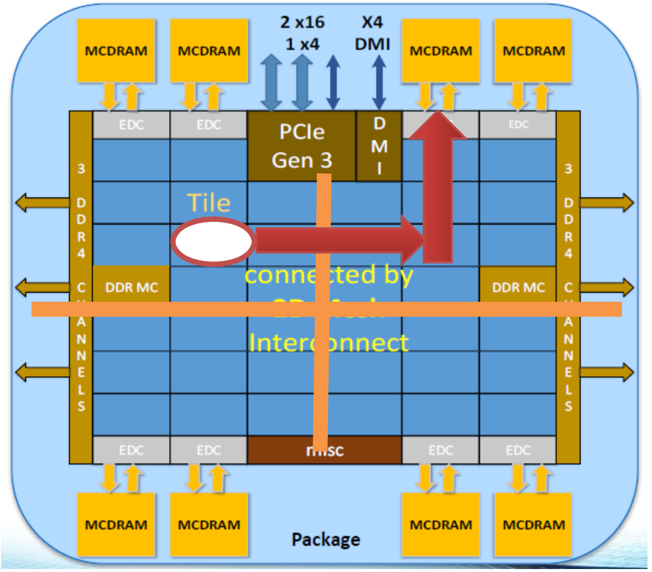
Execution Modes of KNL



Source: Knights Landing (KNL): 2nd Generation Intel® Xeon Phi™ Processor, Avinash Sodani KNL Chief Architect Senior Principal Engineer, Intel Corp.

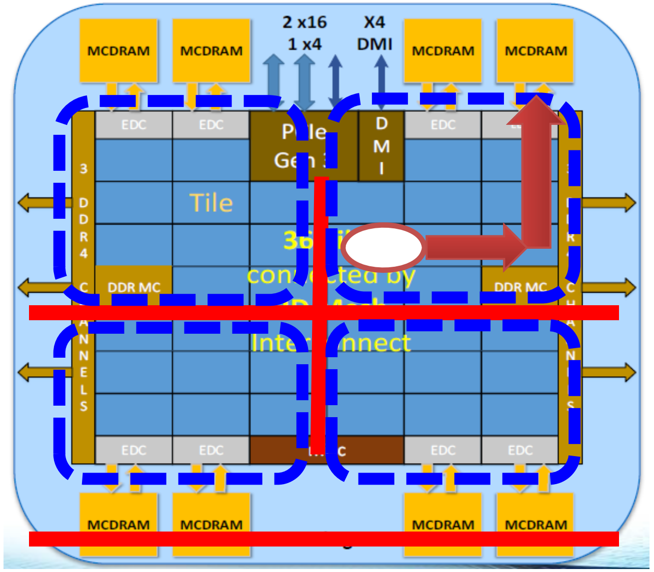
Mesh Modes of KNL

Quadrant



- Chip divided into **four virtual Quadrants.**
- Address hashed to a Directory in the same quadrant as the Memory.
- Affinity between the Directory and Memory.

Sub-NUMA Clustering (SNC)



- Each Quadrant (Cluster) exposed as **a separate NUMA domain** to OS.
- Looks analogous to 4-Socket Xeon Affinity between Tile, Directory and Memory.
- Local communication. Lowest latency of all modes.
- SW **needs to NUMA optimize** to get benefit.

Source: Knights Landing (KNL): 2nd Generation Intel® Xeon Phi™ Processor, Avinash Sodani KNL Chief Architect Senior Principal Engineer, Intel Corp.

Memory and Mesh Modes in This Experiments

1. FLAT-QUADRANT
   – Memory Mode: FLAT, Mesh Mode: QUADRANT
2. FLAT-SNC4
   – Memory Mode: FLAT, Mesh Mode: SNC with 4 clusters
3. CACHE-QUADRANT
   – Memory Mode: CACHE, Mesh Mode: QUADRANT
4. CACHE-SNC4
   – Memory Mode: CACHE, Mesh Mode: SNC with 4 clusters

- NUMA affinity is set by appropriate manner.
- Arrays set in DDR4 in CACHE mode.

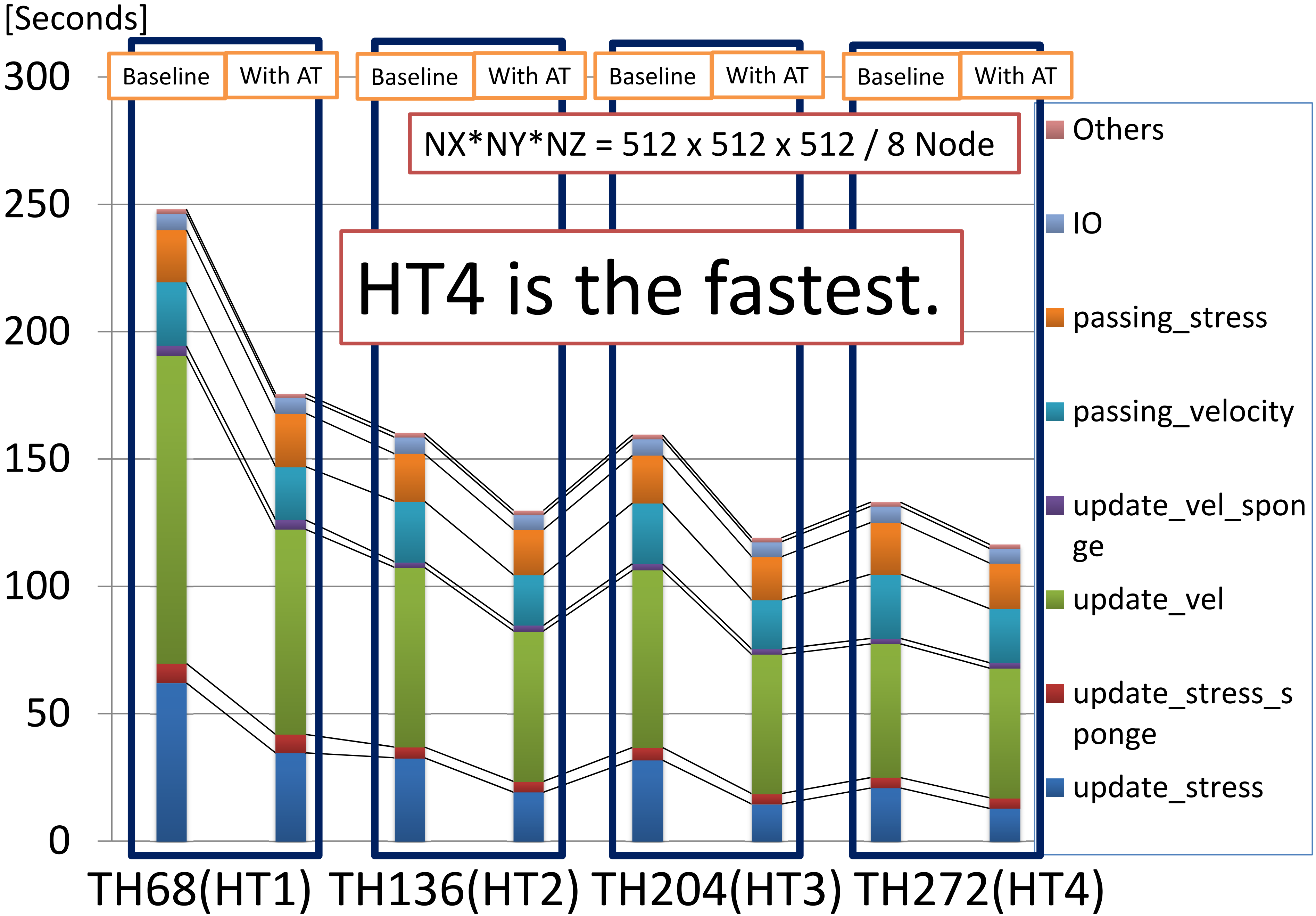
Execution Details

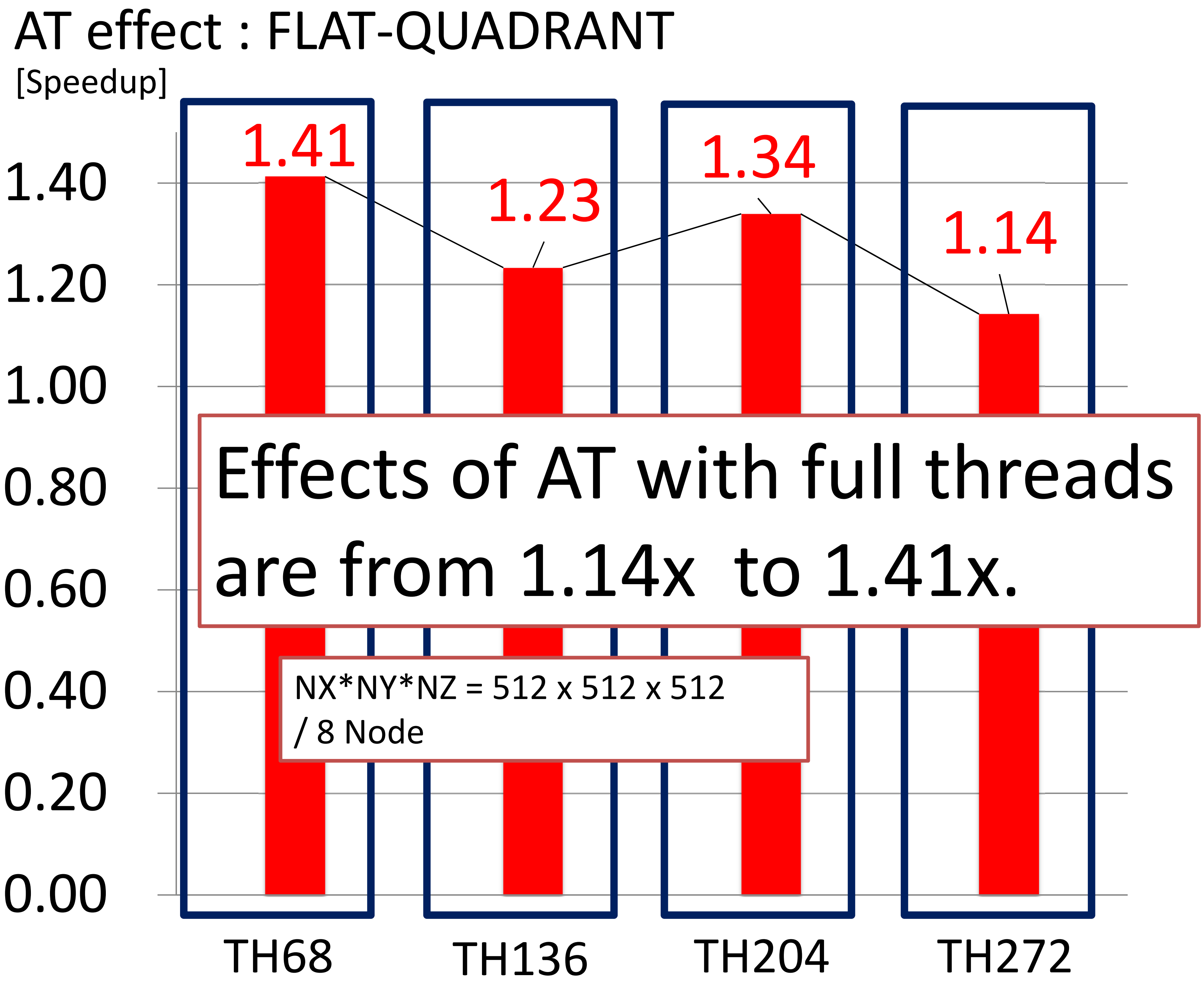
- ppOpen-APPL/FDM ver.0.2
- ppOpen-AT ver.0.2
- The number of time step: 2000 steps
- The number of nodes: 8 node
- Target Problem Size (Almost maximum size with 8 GB/node)
  - NX * NY * NZ = 512 x 512 x 512 / 8 Node
  - NX * NY * NZ = 256 * 256 * 256 / node (!= per MPI Process)
- Target MPI Processes and Threads on the Xeon Phi
  - 1 node of the KNL with 4 HTs (Hyper Threading)
    - **We checked performance of H1-H4, then the H4 is the fastest.**
  - P*X*T*Y*: *X* MPI Processes and *Y* Threads per process
  - P8T272 : Minimum Hybrid MPI-OpenMP execution for ppOpen-APPL/FDM, since it needs minimum 8 MPI Processes.
  - P16T136, P32T68, P64T34, P128T17, P256T8, P512T4, P1024T2
  - P2048T1: pure MPI
- The number of iterations for the kernels: 100

名古屋大学 NAGOYA UNIVERSITY ITC

EFFECT OF HYPER THREADINGS WITH FULL THREADS EXECUTION PER NODE

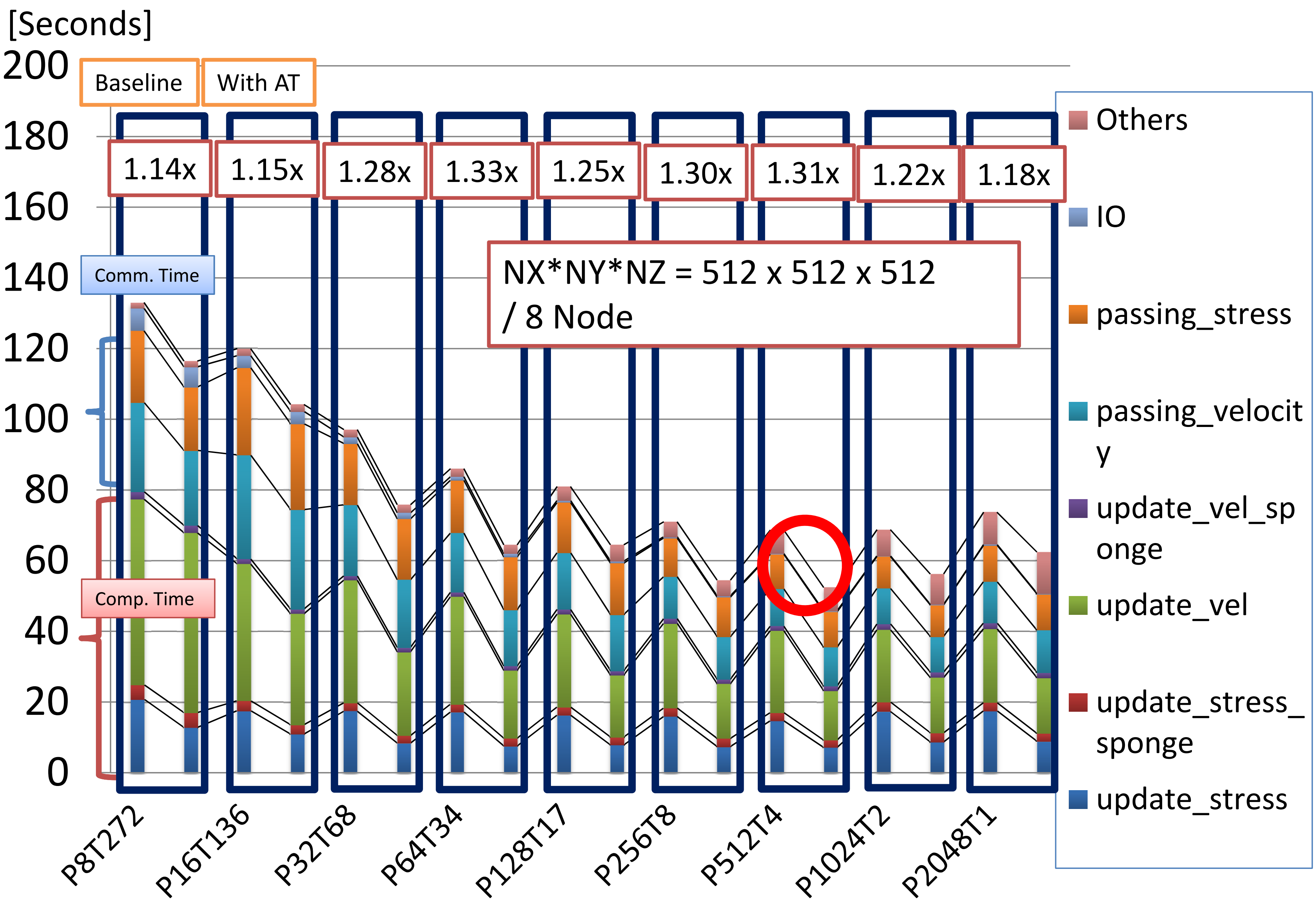
Whole Time（2000 Time Steps）:FLAT-QUADRANT



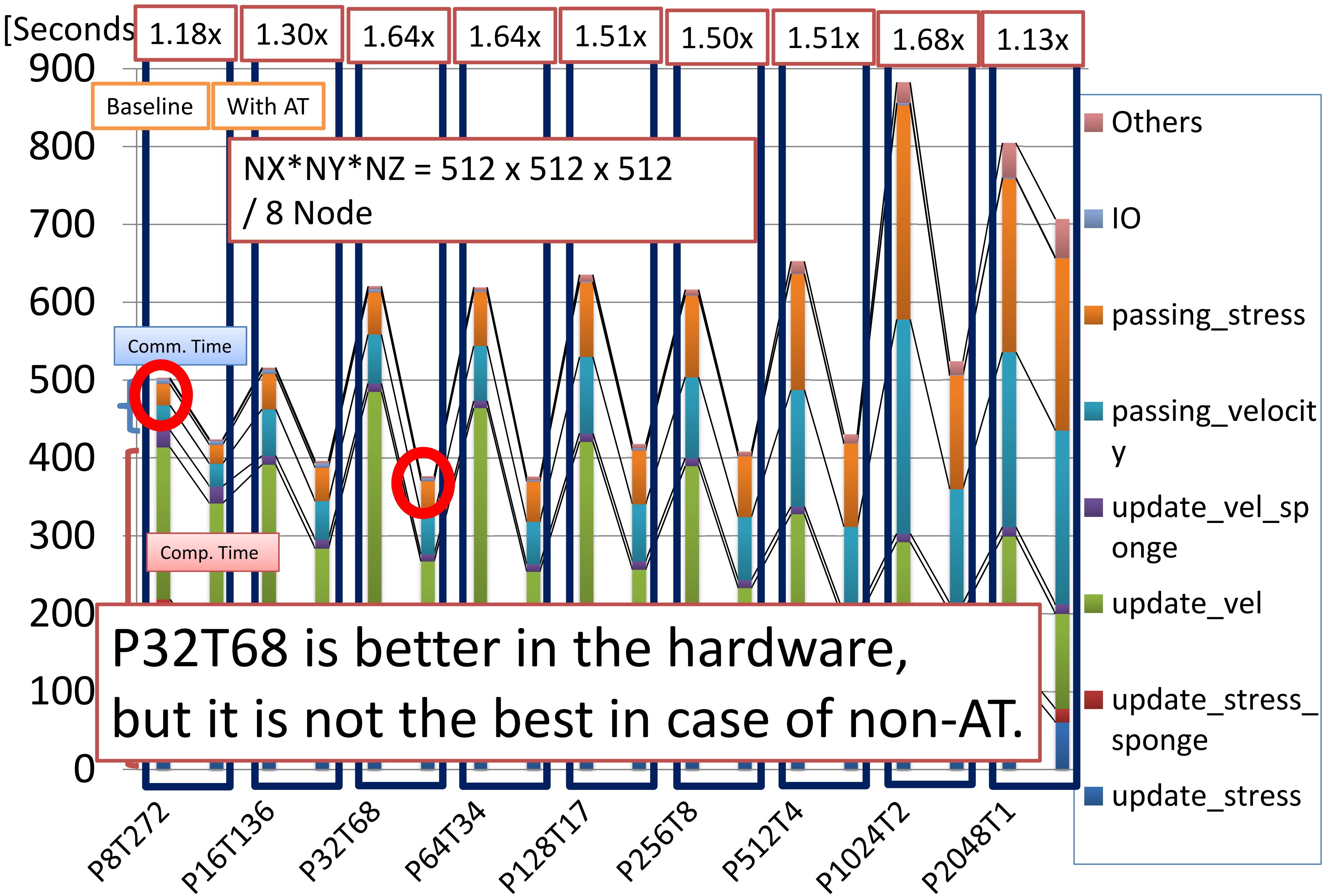

AT effect : FLAT-QUADRANT
[Speedup]
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
1.41
1.23
1.34
1.14
Effects of AT with full threads are from 1.14x to 1.41x.
NX*NY*NZ = 512 x 512 x 512
/ 8 Node
TH68
TH136
TH204
TH272

RESULTS OF HYBRID MPI / OPENMP WITH HT4

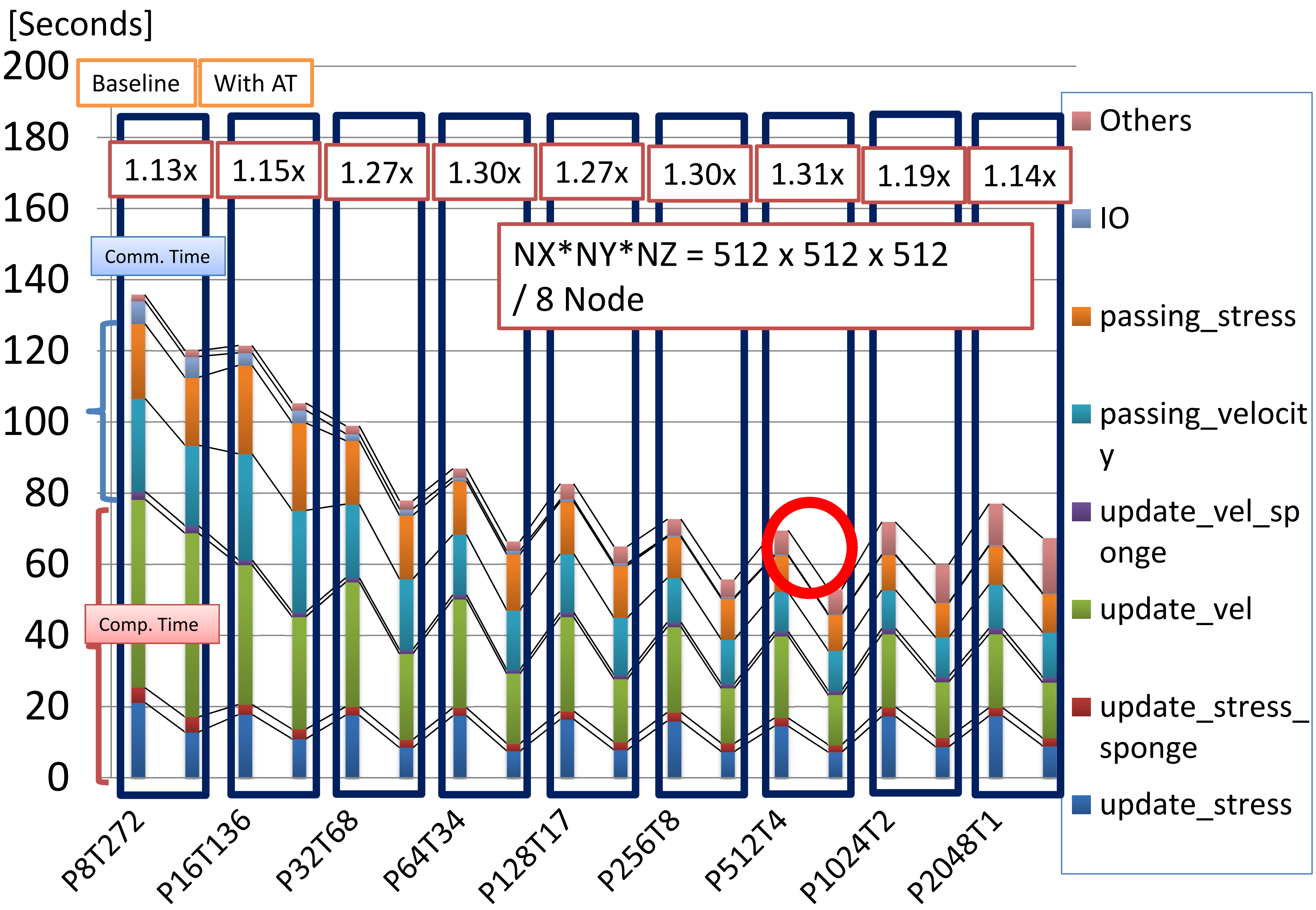
Whole Time（2000 Time Steps）:FLAT-QUADRANT



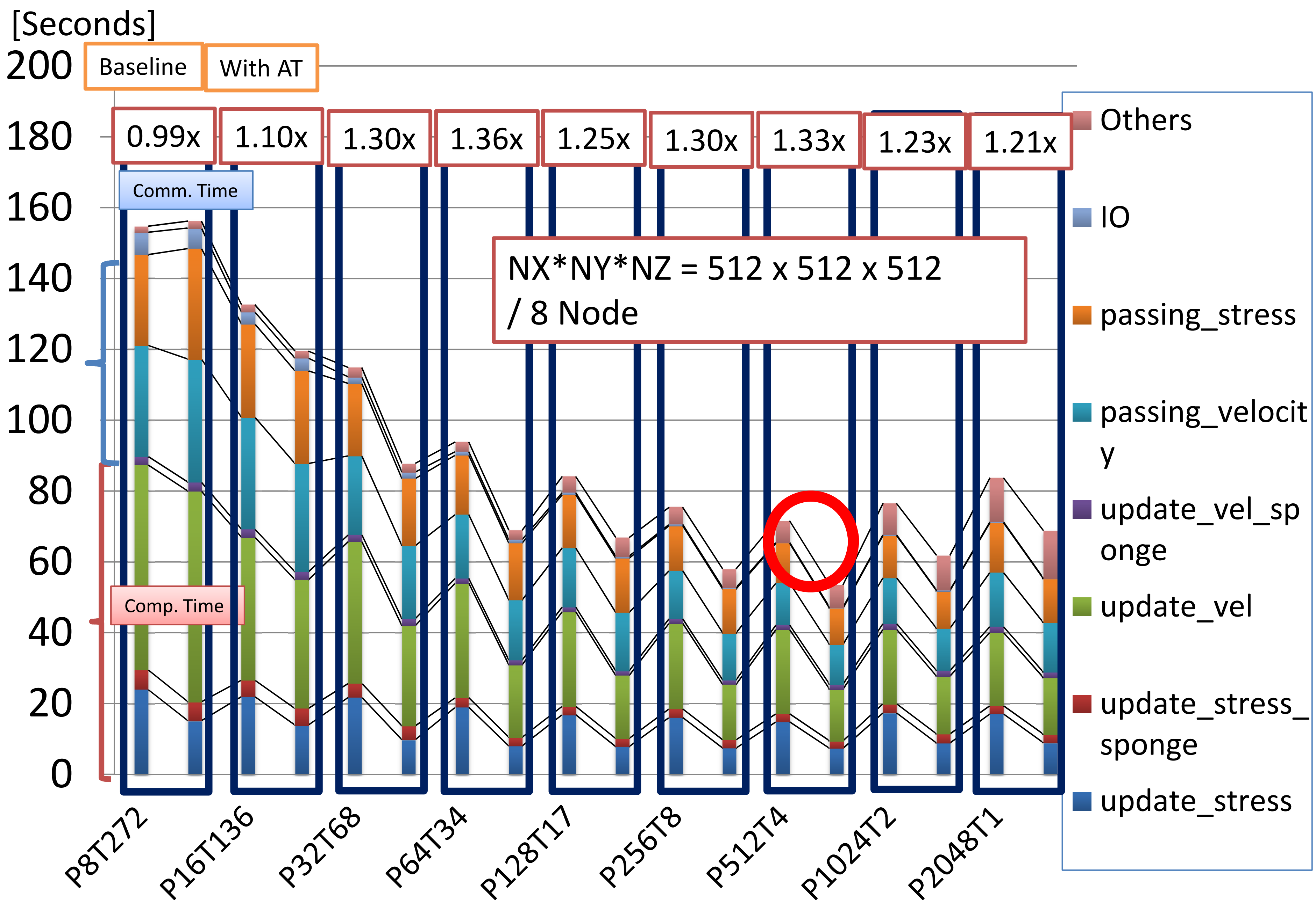
Whole Time（2000 Time Steps）:FLAT-SNC4



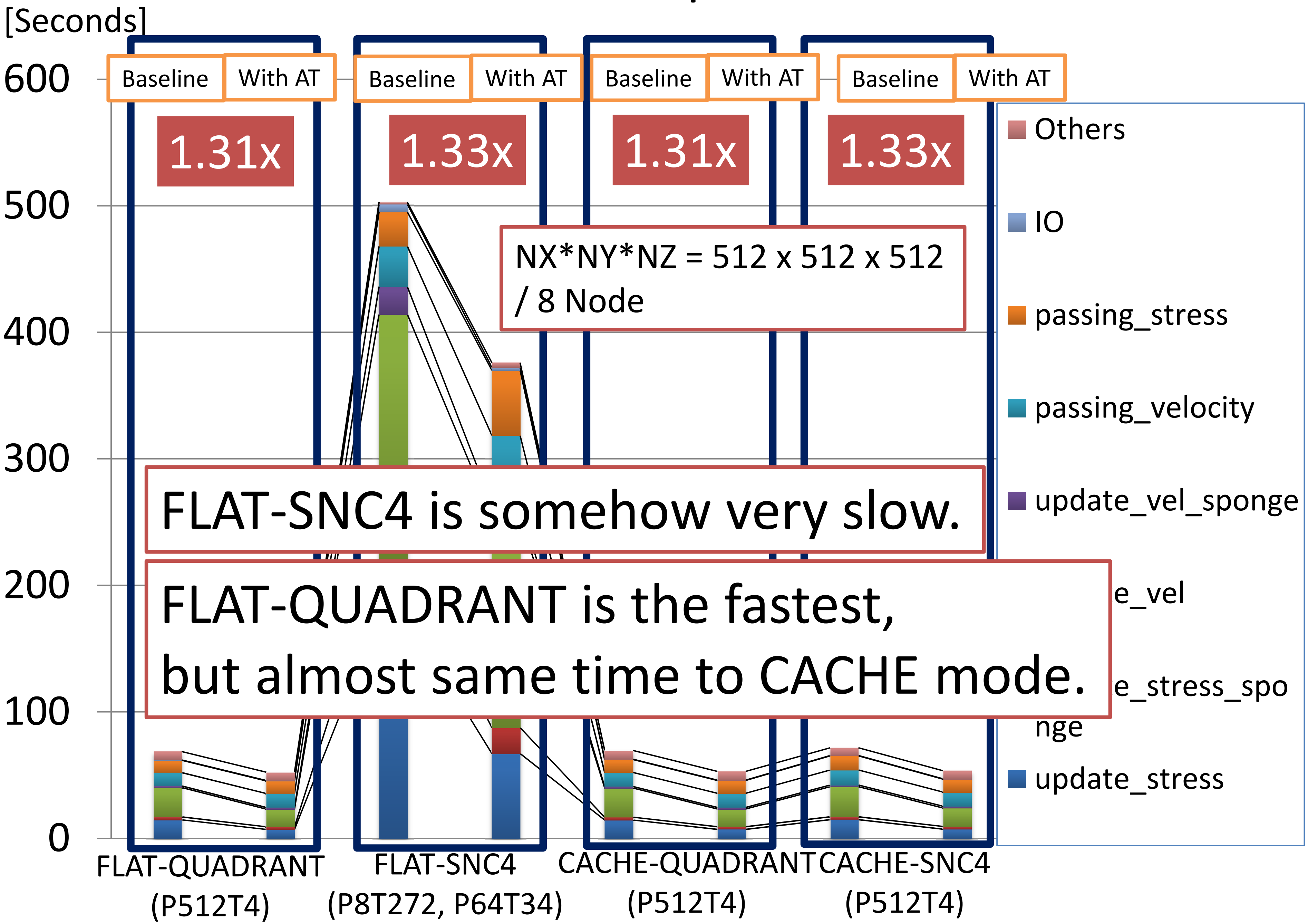
Whole Time（2000 Time Steps）:CACHE-QUADRANT



Whole Time（2000 Time Steps）:CACHE-SNC4

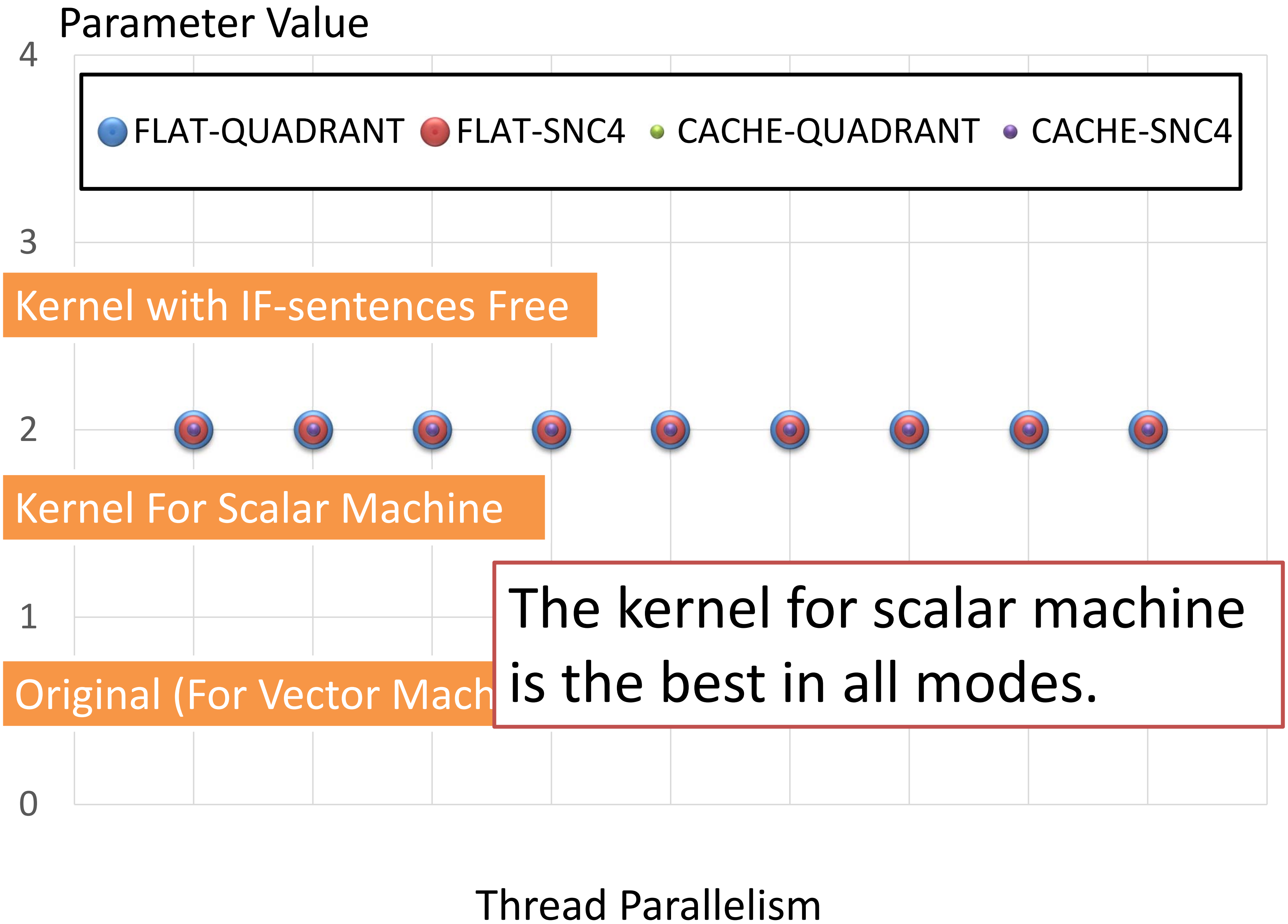


Whole Time（2000 Time Steps）:The Best



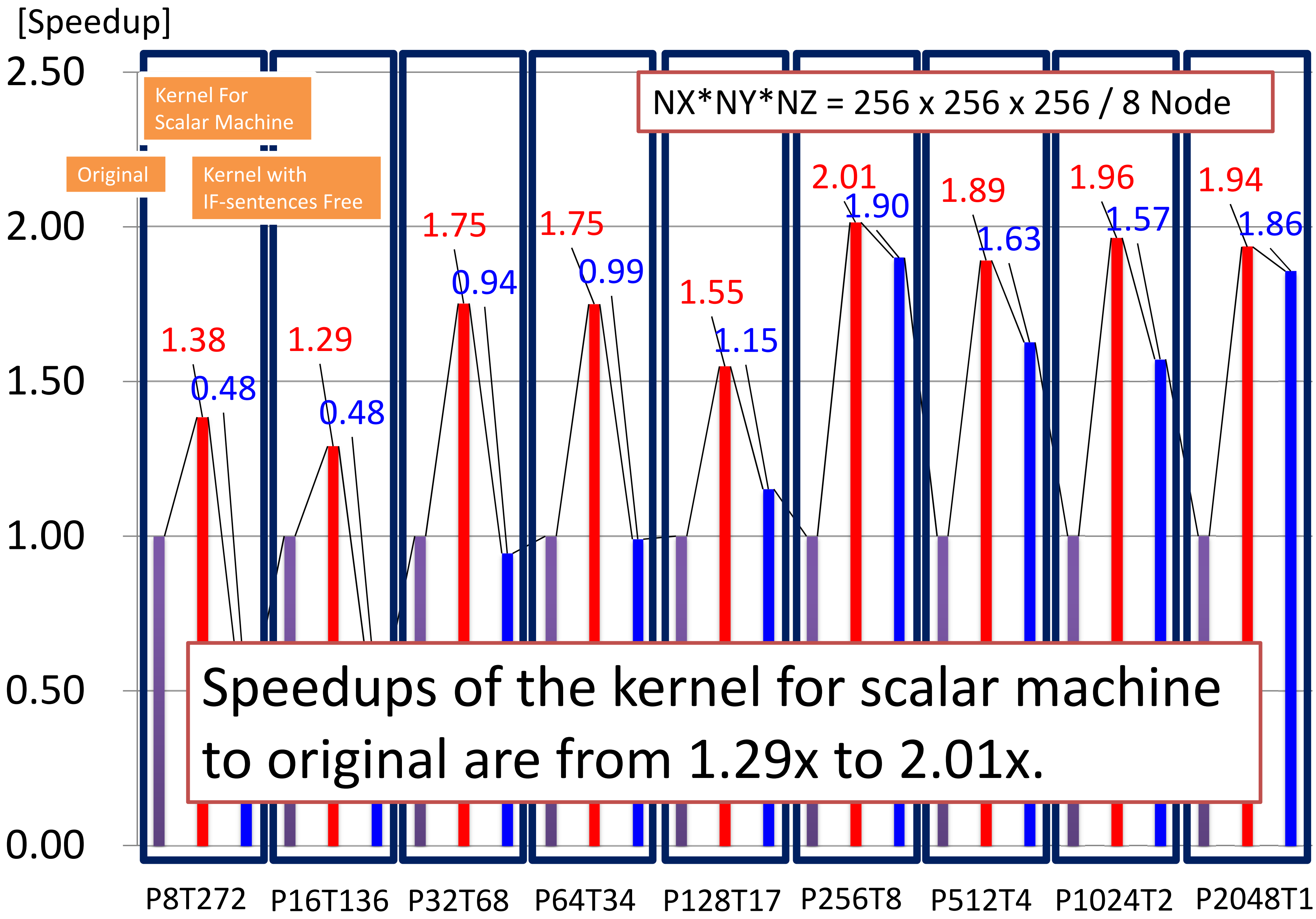
PARAMETER DISTRIBUTION

Parameter Distribution (update_stress) with 8 nodes



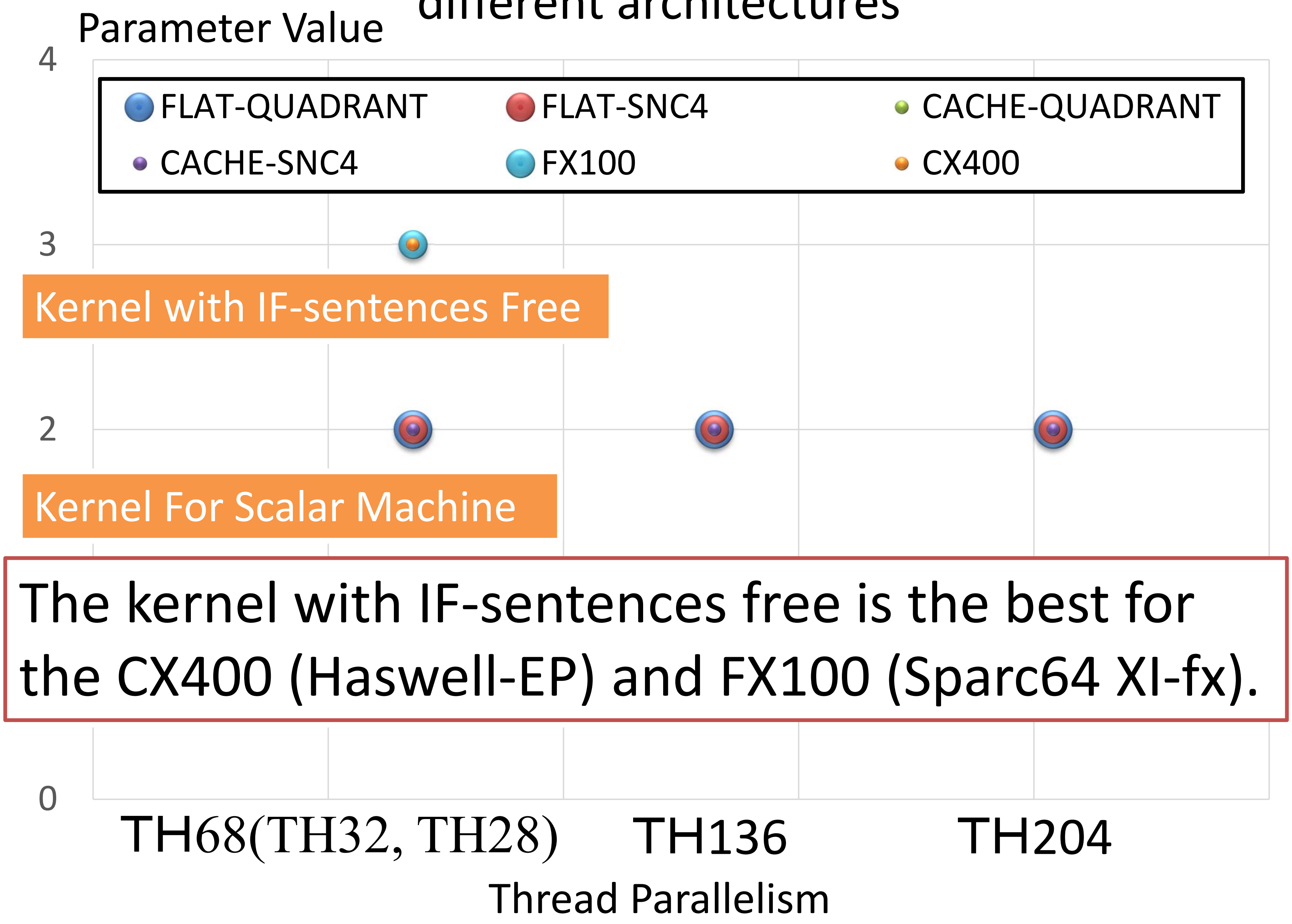
The kernel for scalar machine is the best in all modes.

Kernel speedup (update_stress):FLAT-QUADRANT

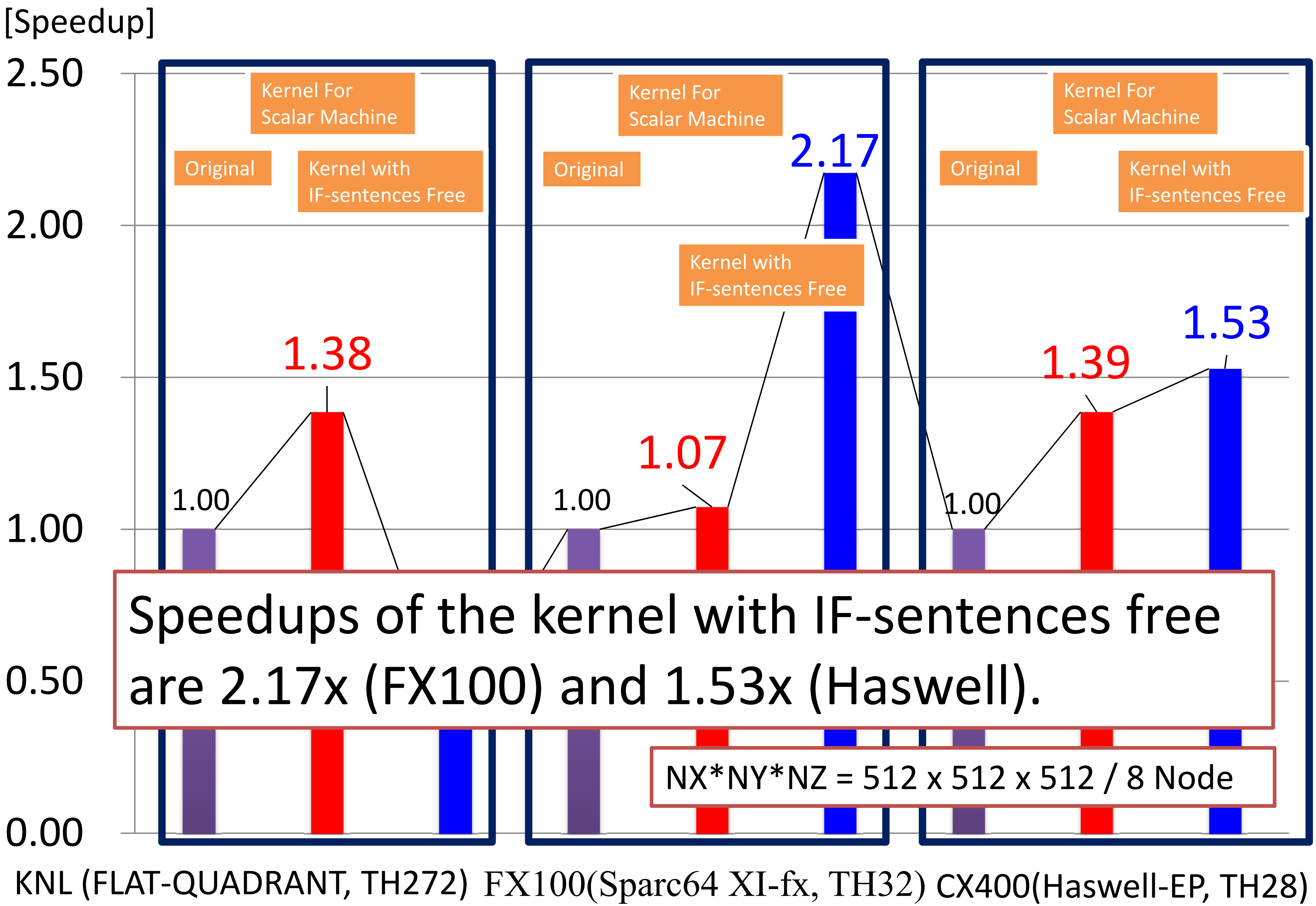


Speedups of the kernel for scalar machine to original are from 1.29x to 2.01x.

Parameter Distribution (update_stress) with 8 nodes in different architectures



Kernel speedup (update_stress, the Best)



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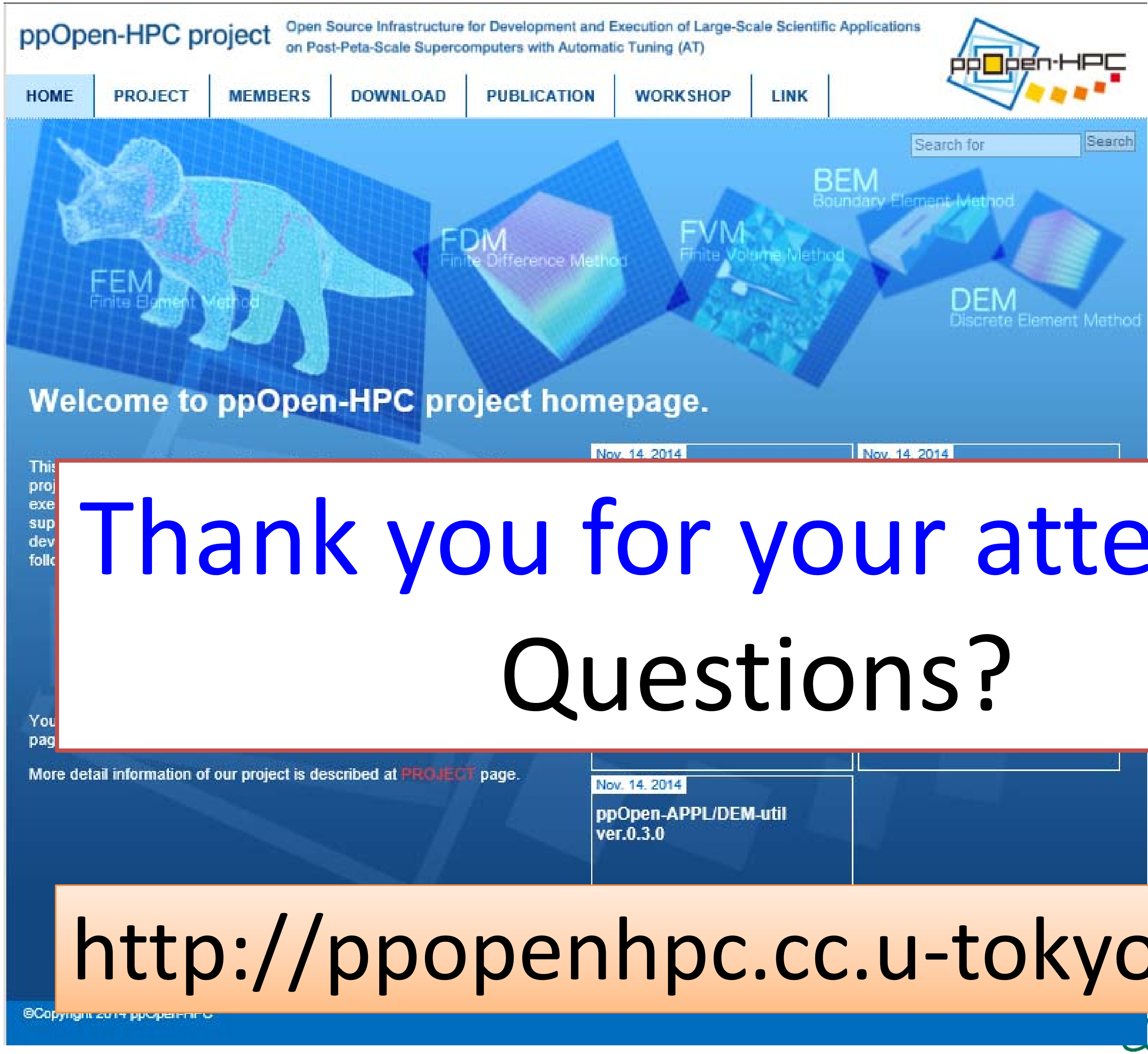
Conclusion Remarks

- We have checked performance of AT with an FDM code with KNL.
- CACHE mode is not slow with compared to FLAT mode.
- Sub-NUMA Clustering (SNC) mode in FLAT mode is somehow very slow.
  - We do not find the reason yet.
- We also observe big difference according to type of MPI/OpenMP executions by increasing the number of MPI processes.

  -> We still need to tune the type of MPI-OpenMP in advanced multicore CPU.

Future Work

- Find the reason that why FLAT-SNC4 is very slow.
- Find methodology (or novel implementations) to maximize performance w.r.t NUMA affinity in KNL.
- Implement a new AT facility (and model the performance) w.r.t NUMA affinity in KNL.



Thank you for your attention!

Questions?

http://ppopenhpc.cc.u-tokyo.ac.jp/