Towards a Computationally Bound Numerical Weather Prediction Model

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Definitions

- Computationally bound:
  - A significant portion of processing time is spent doing floating point operations (FLOPS)
- Memory Bound:
  - A significant amount of processing time is spent waiting for data from memory

Why should you care about Weather Forecasting and Computational Efficiency?

Because weather forecast are time critical!

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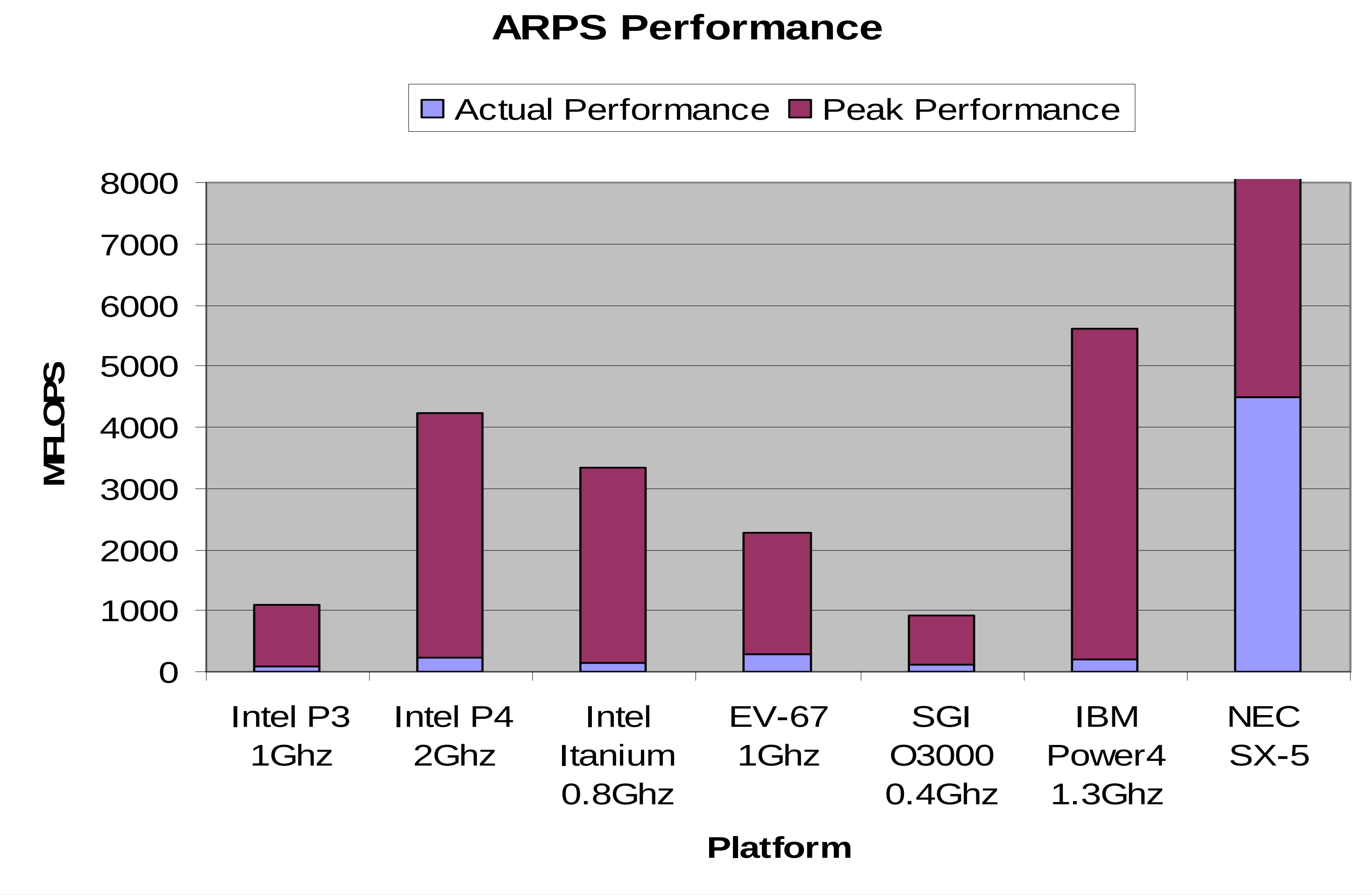
Benchmarks



ARPS Performance
Actual Performance
Peak Performance
MFLOPS
8000
7000
6000
5000
4000
3000
2000
1000
0
Intel P3 1Ghz
Intel P4 2Ghz
Intel Itanium 0.8Ghz
EV-67 1Ghz
SGI O3000 0.4Ghz
IBM Power4 1.3Ghz
NEC SX-5
Platform

The Problem

- Poor efficiency of Numerical Weather Prediction (NWP) models on modern supercomputers degrades the quality of the forecast to the public

The Future

- Multicore technology:
  - Many cores (individual cpu’s) access main memory via one common pipeline
- Reduce the bandwidth to each core
- Will produce memory bound code whose performance enhancements will be tied to the memory speed, not processing speed (yikes!!!!!)

Forecast Quality

- Forecast quality is a function of grid spacing/feature resolution (more grid points are better)
- Forecasts using 2 times more grid points in each direction requires 16 times more processing power!!!

The Goal

- Use the maximum number of grid points
- Obtain a computationally bound model

- Result: produce better forecasts faster!

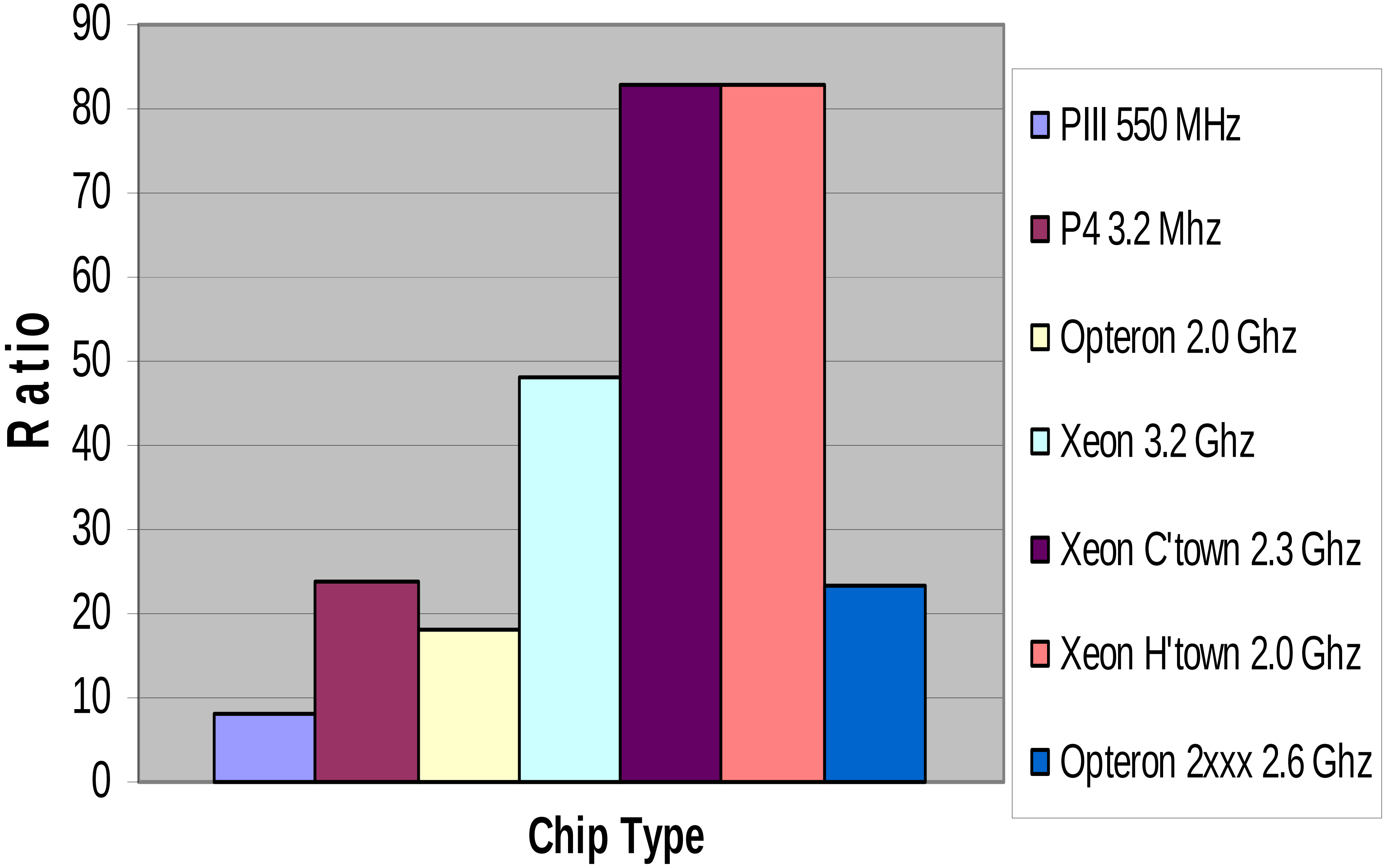
Tools

- Code analysis:
  - Count arrays – assess memory requirements
  - Calculations
  - Data reuse etc
  - Solution techniques (spatial and time differencing methods
- Use PAPI (Performance Application Programming Interface) to track FLOPS/cache misses etc
- Define metrics for evaluating solution techniques and predict results

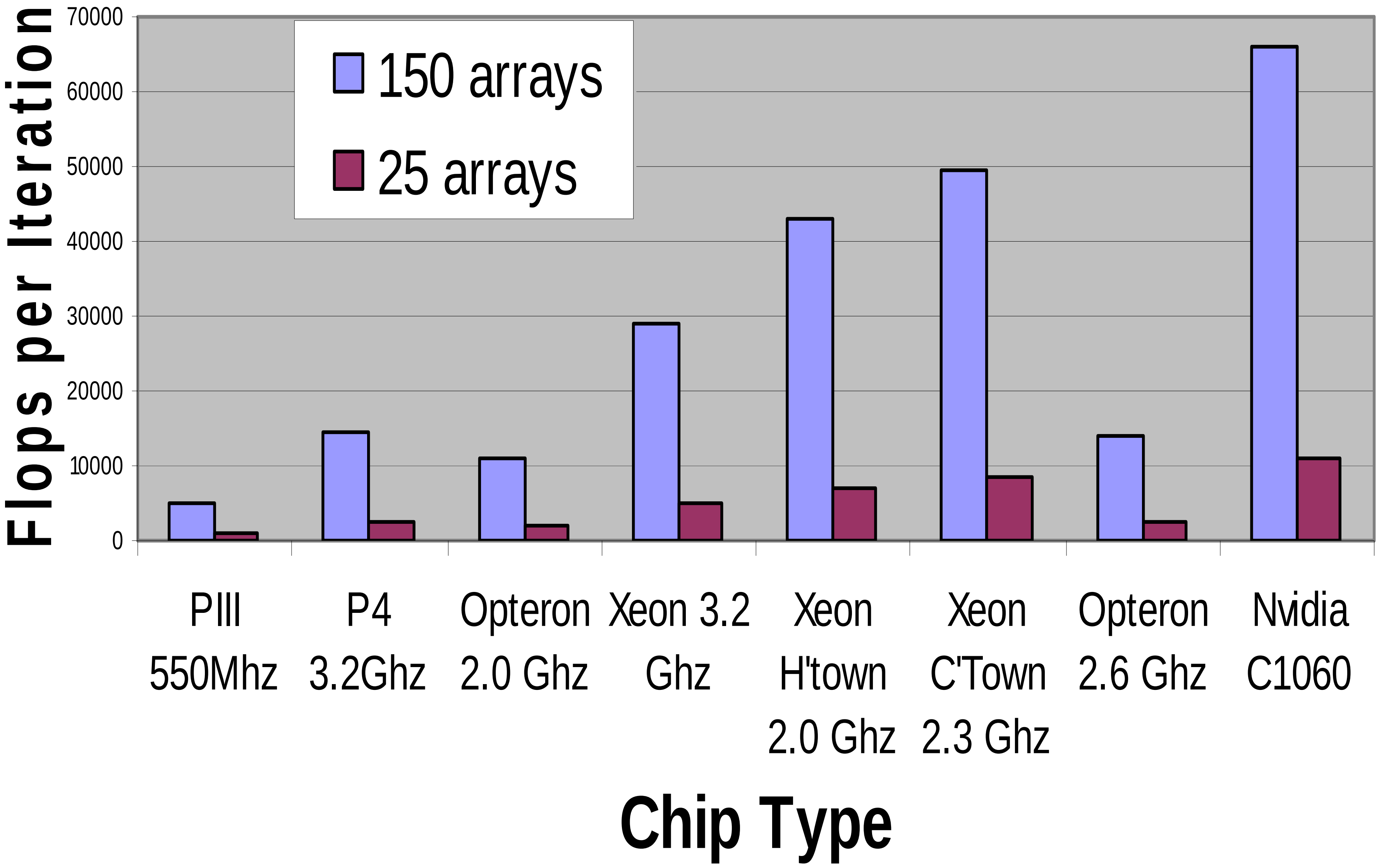
Metrics

- Single precision flop to memory bandwidth ratio
  - peak flop rating/peak main memory bandwidth
- Actual bandwidth needed to achieve peak flop rate (simple multiply: a = b*c)
  - 4bytes/variable*3variables/flop*flops/clock*clock /sec
- Flops needed to cover the time required to load data from memory
  - #of 3-D arrays *4bytes/array * required peak flop bandwidth

Peak Flop/Memory Bandwidth



Flops Required for Weather Code to Keep Processor Busy As a Function of Memory Usage



Research Weather Model

- 61 3-D arrays (including 11 temporary arrays (ARPS/WRF has ~150 3-D arrays)
- 1200 flops per/cell/iteration (1 big/small step)
- 3-time levels required for time dependant variables
- Split-time steps
  - Big time step (temperature, advection, mixing)
  - Small time step (winds, pressure)

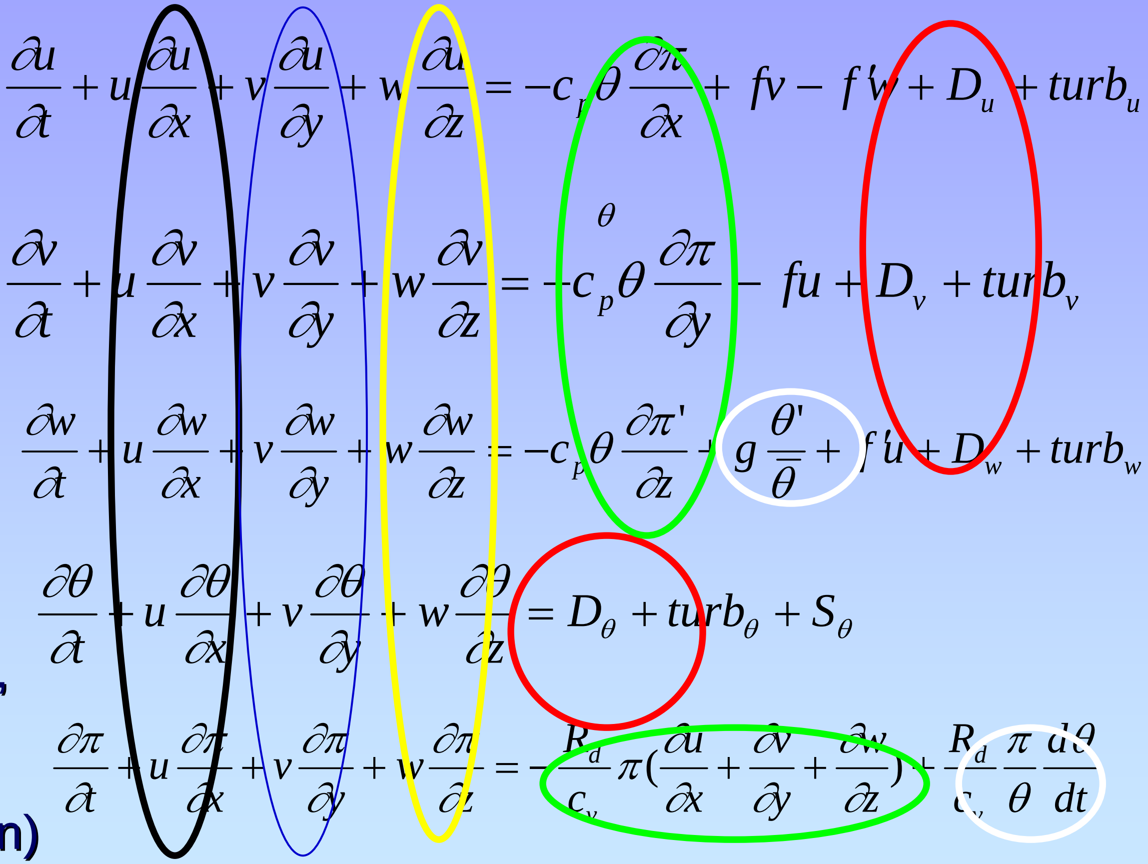
Result: ~5% of peak performance…

Solution Approach

- Compute computational and turbulent mixing terms for all variables except pressure
- Compute advection forcing for all variables
- Compute pressure gradient and update variables

Weather Model Equations (PDE’s)

- U,V,W represent winds
- Theta θ represents temperature
- Pi π represents pressure
- T – Time
- X – east west direction
- Y – north south direction
- Z – vertical direction
- Turb – turbulence terms (what can’t be measured/predicted)
- S – Source terms, condensation, evaporation, heating, cooling
- D – numerical smoothing
- f – Coriolis force (earth’s rotation)



$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -c_p\theta\frac{\partial \pi}{\partial x} + fv - f'w + D_u + turb_u$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\overset{\theta}{c}_p\theta\frac{\partial \pi}{\partial y} - fu + D_v + turb_v$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -c_p\theta\frac{\partial \pi'}{\partial z} + g\frac{\theta'}{\overline{\theta}} + f'u + D_w + turb_w$$

$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + w\frac{\partial \theta}{\partial z} = D_\theta + turb_\theta + S_\theta$$

$$\frac{\partial \pi}{\partial t} + u\frac{\partial \pi}{\partial x} + v\frac{\partial \pi}{\partial y} + w\frac{\partial \pi}{\partial z} = -\frac{R_d}{c_v}\pi\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + \frac{R_d}{c_v}\frac{\pi}{\theta}\frac{d\theta}{dt}$$

Code Analysis Results

- Memory usage:
  - 3 time levels for each predicted variable
  - 11 temporary arrays (1/5 of the memory)
- Solution process breaks calculations up into several sections
  - Compute one term thru the entire grid and then compute the next term
- Tiling can help improve the cache reuse but did not make a big difference

Previous Results

- Cache misses were significant
- Need to reduce cache misses via:
  - Reduction in overall memory requirements
  - Increase operations per memory reference
  - Simplify the code (if possible)

Think outside the box

- Recipe:
  - Not getting acceptable results? (~5% peak)
  - Develop useful metrics
  - Check the compiler options
  - Other numerical solution methods
  - Using simple loops to achieve peak performance on an instrumented platform
  - Then apply the results to the full scale model

Revised Code

- New time scheme to reduce memory footprint (RK3, no time splitting!)
  - Reduces memory requirements by 1 3-D array per time dependant variable (reduces footprint by 8 arrays)
  - More accurate (3rd order vs 1st order)
- Combine ALL computations into one loop (or directional loops)
  - Removes need for 11 temporary arrays

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$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -c_p\theta\frac{\partial \pi}{\partial x} + fv - f'w + D_u + turb_u$$

$$\theta$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -c_p\theta\frac{\partial \pi}{\partial y} - fu + D_v + turb_v$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -c_p\theta\frac{\partial \pi'}{\partial z} + g\frac{\theta'}{\bar{\theta}} + f'u + D_w + turb_w$$

$$\frac{\partial \pi}{\partial t} + u\frac{\partial \pi}{\partial x} + v\frac{\partial \pi}{\partial y} + w\frac{\partial \pi}{\partial z} = -\frac{R_d}{c_v}\pi\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + \frac{R_d}{c_v}\frac{\pi}{\theta}\frac{d\theta}{dt}$$

$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + w\frac{\partial \theta}{\partial z} = D_\theta + S_\theta + turb_\theta$$

Revised Solution Technique

- Reuses data
- Reduces intermediate results and loads to/from memory
- Sample loops:

2^{nd} Order U-Velocity Update

```
call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
 DO k=2,nz-2  ! scalar limits  u(2) is the q's/forcing.
 DO j=2,ny-1  ! scalar limits u(1) is the
              !  updated/previous u
DO i=2,nx-1 ! vector limits
     u(i,j,k,2)=-u(i,j,k,2)*rk_constant
   c  e-w adv
      :     -tema*((u(i+1,j,k,1)+u(i,j,k,1))*
      :             (u(i+1,j,k,1)-u(i,j,k,1))
      : +  (u(i,j,k,1)+u(i-1,j,k,1))* (u(i,j,k,1)-u(i-1,j,k,1)))
   c  n-s adv
      :     -temb*((v(i,j+1,k,1)+v(i-1,j+1,k,1))*
      :             (u(i,j+1,k,1)-u(i,j,k,1))
      : +  (v(i,j,k,1)+v(i-1,j,k,1))* (u(i,j,k,1)-u(i,j-1,k,1)))
   c  vert adv
      :     -temc*((w(i,j,k+1,1)+w(i-1,j,k+1,1))*
      :             (u(i,j,k+1,1)-u(i,j,k,1))
      : + (w(i,j,k,1)+w(i-1,j,k,1))*(u(i,j,k,1)-u(i,j,k-1,1)))
   c  pressure gradient
      :      -temd*(ptrho(i,j,k)+ptrho(i-1,j,k))*
      :                  (pprt(i,j,k,1)-pprt(i-1,j,k,1))
   c  compute the second order cmix x terms.
      :       + temg*(((u(i+1,j,k,1)-ubar(i+1,j,k))-
      :                (u(i,j,k,1)-ubar(i,j,k)))-
      :  ((u(i,j,k,1)-ubar(i,j,k))- (u(i-1,j,k,1)-ubar(i-1,j,k))))
```

```
ontinuedL
     c compute the second order cmix y terms.
      :       + temh*(((u(i,j+1,k,1)-ubar(i,j+1,k))-
      :                (u(i,j,k,1)-ubar(i,j,k)))-
      :               ((u(i,j,k,1)-ubar(i,j,k))-
      :                (u(i,j-1,k,1)-ubar(i,j-1,k))))
     c compute the second order cmix z terms.
      :       + temi*(((u(i,j,k+1,1)-ubar(i,j,k+1))-
      :                (u(i,j,k,1)-ubar(i,j,k)))-
      :               ((u(i,j,k,1)-ubar(i,j,k))-
      :                (u(i,j,k-1,1)-ubar(i,j,k-1))))
          END DO   ! 60 calculations...
        END DO
      END DO
      call PAPIF_flops(real_time, cpu_time, fp_ins,
      mflops, ierr)
      print *,'2nd order u'
      write (*,101) nx, ny,nz,
     +            real_time, cpu_time, fp_ins, mflops
```

60 flops/7 arrays

4th order U-Velocity uadv/mix

```
     call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
      DO k=2,nz-2  ! scalar limits  u(2) is the q's/forcing.
        DO j=2,ny-2 ! scalar limits u(1) is the updated/previous u
          DO i=3,nx-2
            u(i,j,k,2)=-u(i,j,k,2)*rk_constant1(n)
c  e-w adv
     :  -tema*((u(i,j,k,1)+u(i+2,j,k,1))*(u(i+2,j,k,1)-u(i,j,k,1))
     :        +(u(i,j,k,1)+u(i-2,j,k,1))*(u(i,j,k,1)-u(i-2,j,k,1)))
     :  +temb*((u(i+1,j,k,1)+u(i,j,k,1))*(u(i+1,j,k,1)-u(i,j,k,1))
     :       + (u(i,j,k,1)+u(i-1,j,k,1))*(u(i,j,k,1)-u(i-1,j,k,1)))
  :  -tema*(((((u(i+2,j,k,1)-ubar(i+2,j,k))-(u(i+1,j,k,1)-ubar(i+1,j,k)))-
     :           ((u(i+1,j,k,1)-ubar(i+1,j,k))-(u(i,j,k,1)-ubar(i,j,k))))-
     :          (((u(i+1,j,k,1)-ubar(i+1,j,k))-(u(i,j,k,1)-ubar(i,j,k)))-
     :           ((u(i,j,k,1)-ubar(i,j,k))-(u(i-1,j,k,1)-ubar(i-1,j,k)))))-
     :         ((((u(i+1,j,k,1)-ubar(i+1,j,k))-(u(i,j,k,1)-ubar(i,j,k)))-
     :           ((u(i,j,k,1)-ubar(i,j,k))-(u(i-1,j,k,1)-ubar(i-1,j,k))))-
     :          (((u(i,j,k,1)-ubar(i,j,k))- (u(i-1,j,k,1)-ubar(i-1,j,k)))-
     :           ((u(i-1,j,k,1)-ubar(i-1,j,k))-(u(i-2,j,k,1)-ubar(i-2,j,k))))))
        END DO’s
      Print PAPI results...
```

52 flops/3 arrays

4th order W wadv/mix Computation

```
    call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
    DO k=3,nz-2   ! limits 3,nz-2
      DO j=1,ny-1
        DO i=1,nx-1
          w(i,j,k,2)=w(i,j,k,2)
c  vert adv fourth order
    : +tema*((w(i,j,k,1)+w(i,j,k+2,1))*(w(i,j,k+2,1)-w(i,j,k,1))
    :       +(w(i,j,k-2,1)+w(i,j,k,1))*(w(i,j,k,1)-w(i,j,k-2,1)))
    : -temb*((w(i,j,k-1,1)+w(i,j,k,1))*(w(i,j,k,1)-w(i,j,k-1,1))
    :       +(w(i,j,k+1,1)+w(i,j,k,1))*(w(i,j,k+1,1)-w(i,j,k,1)))
c compute the fourth order cmix z terms.
    :  -tema*((((w(i,j,k+2,1)-w(i,j,k+1,1))-
    :           (w(i,j,k+1,1)-w(i,j,k,1)))-
    :          ((w(i,j,k+1,1)-w(i,j,k,1))- (w(i,j,k,1)-w(i,j,k-1,1))))-
    :         (((w(i,j,k+1,1)-w(i,j,k,1))-(w(i,j,k,1)-w(i,j,k-1,1)))-
    :          ((w(i,j,k,1)-w(i,j,k-1,1))-(w(i,j,k-1,1)-w(i,j,k-2,1)))))
        END DO   ! 35 calculations...
      END DO
    END DO

    call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
    print *,'wadvz'
    write (*,101) nx, ny,nz,
   +             real_time, cpu_time, fp_ins, mflops
```

35 flops/2 arrays

Final U Loop

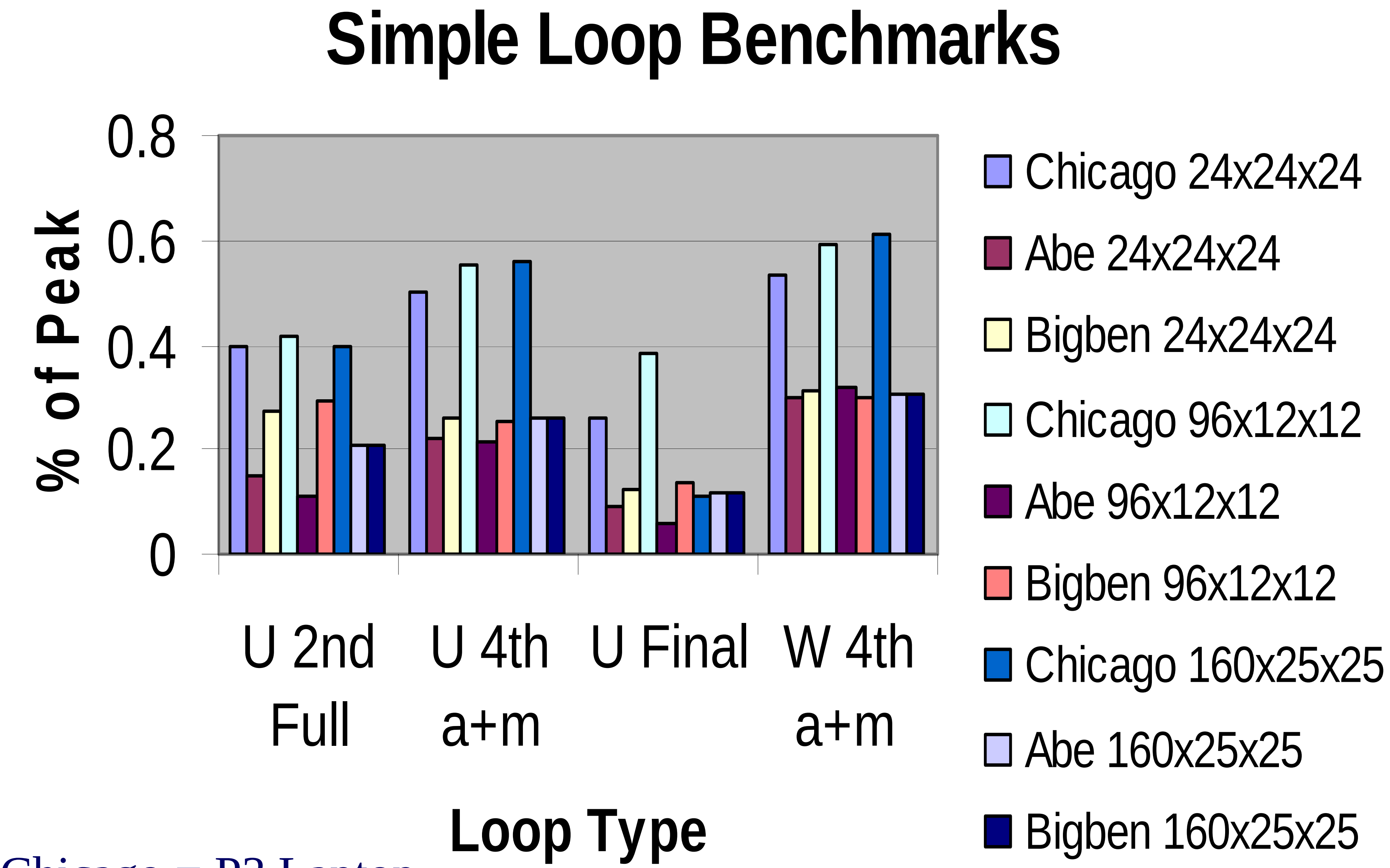
```
 call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
 DO k=2,nz-2    ! complete the u computations
   DO j=2,ny-2
     DO i=2,nx-1
       u(i,j,k,1) = u(i,j,k,1) + u(i,j,k,2)*rk_constant2(n)
     END DO
   END DO
  END DO
 call PAPIF_flops(real_time, cpu_time, fp_ins, mflops, ierr)
 print *,'ufinal'
 write (*,101) nx,ny,nz,
+               real_time, cpu_time, fp_ins, mflops
```

2 flops/2 arrays

Individual Loop Tests

- Hardwired array bounds (due to PGI compiler 3.2 version not optimizing when using dynamic array allocation)
- Prefetching must be specified
- Varied array sizes/memory footprint
- Use 3 loops from 2nd and 4th order (spatial) solution techniques
- Compare flops/timings/metrics

Memory size = 5 arrays *4* nx*ny*nz



Chicago = P3 Laptop

Model Tests

- Current scheme (Klemp-Wilhelmson method) 2nd and 4th order spatial differencing
- RK3 scheme: all computations (except temperature) are computed on the small time step (6x more work is performed in this case as in the current scheme)
- Show results from various platforms as a function of mflops and percent of peak

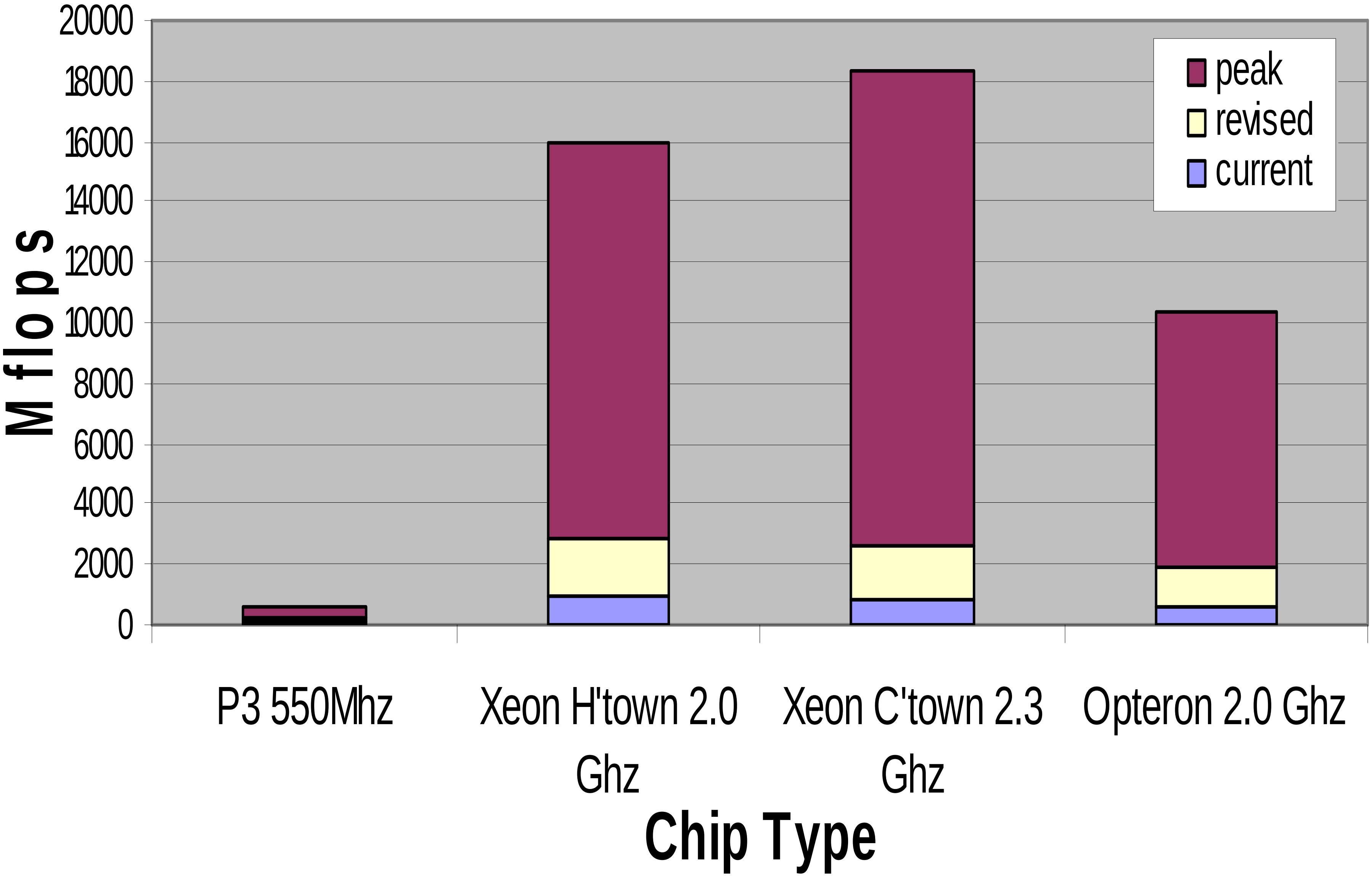
Test Setup

- 5 sec dtbig, 0.5 sec dtsmall
- 1000x1000x250m grid spacing
- 600 second warm bubble simulation
- No turbulence (ok for building scale flow predictions!)
- Dry dynamics only

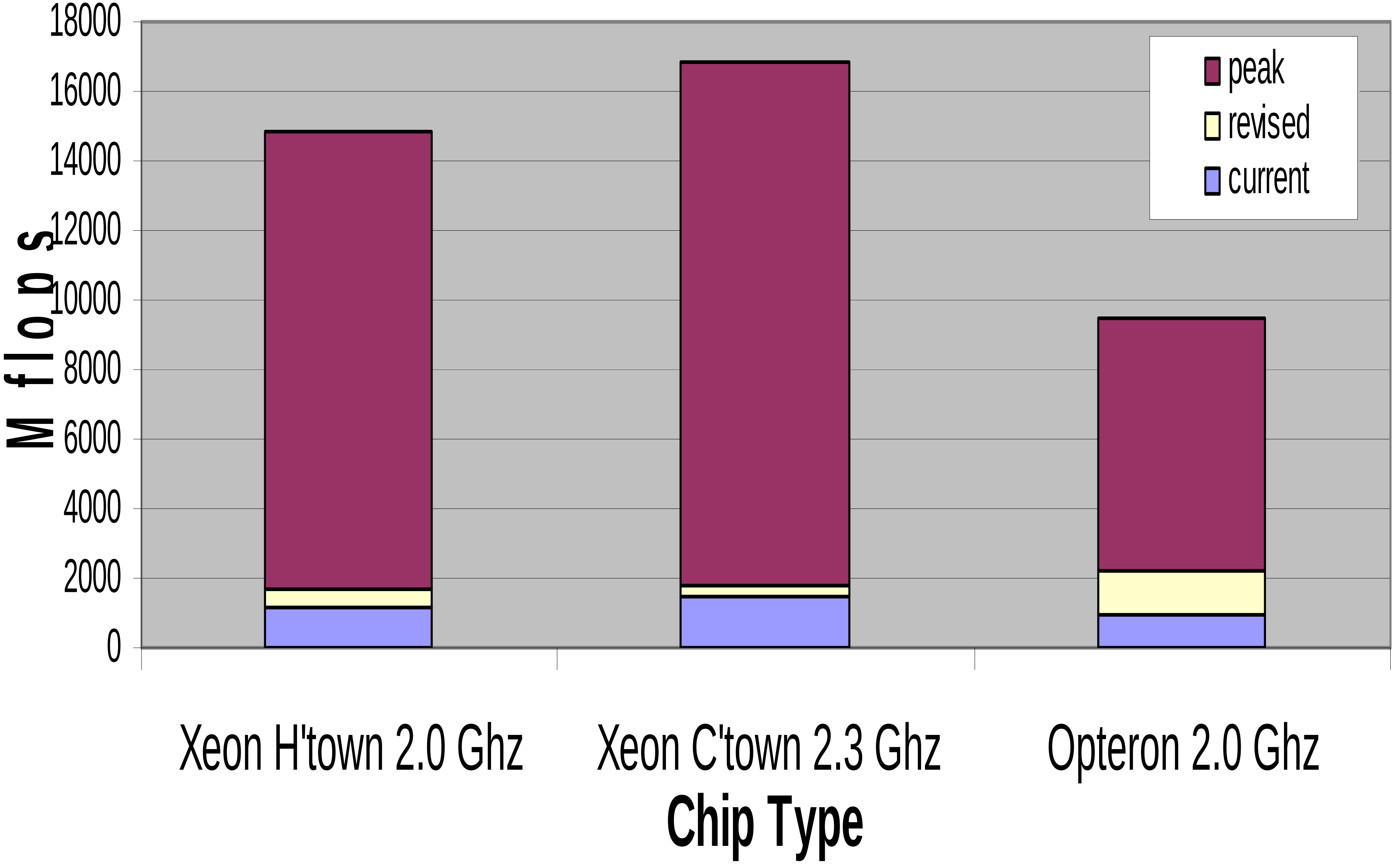
Flop Count/per Iteration

- 4th Order:
  - Current code:
    - 1200 flops (all terms)
    - ~600 flops for these tests
  - Revised code:
    - ~535 flops (w/o terrain, moisture)
- 2nd Order:
  - 260 flops (w/o terrain, moisture)

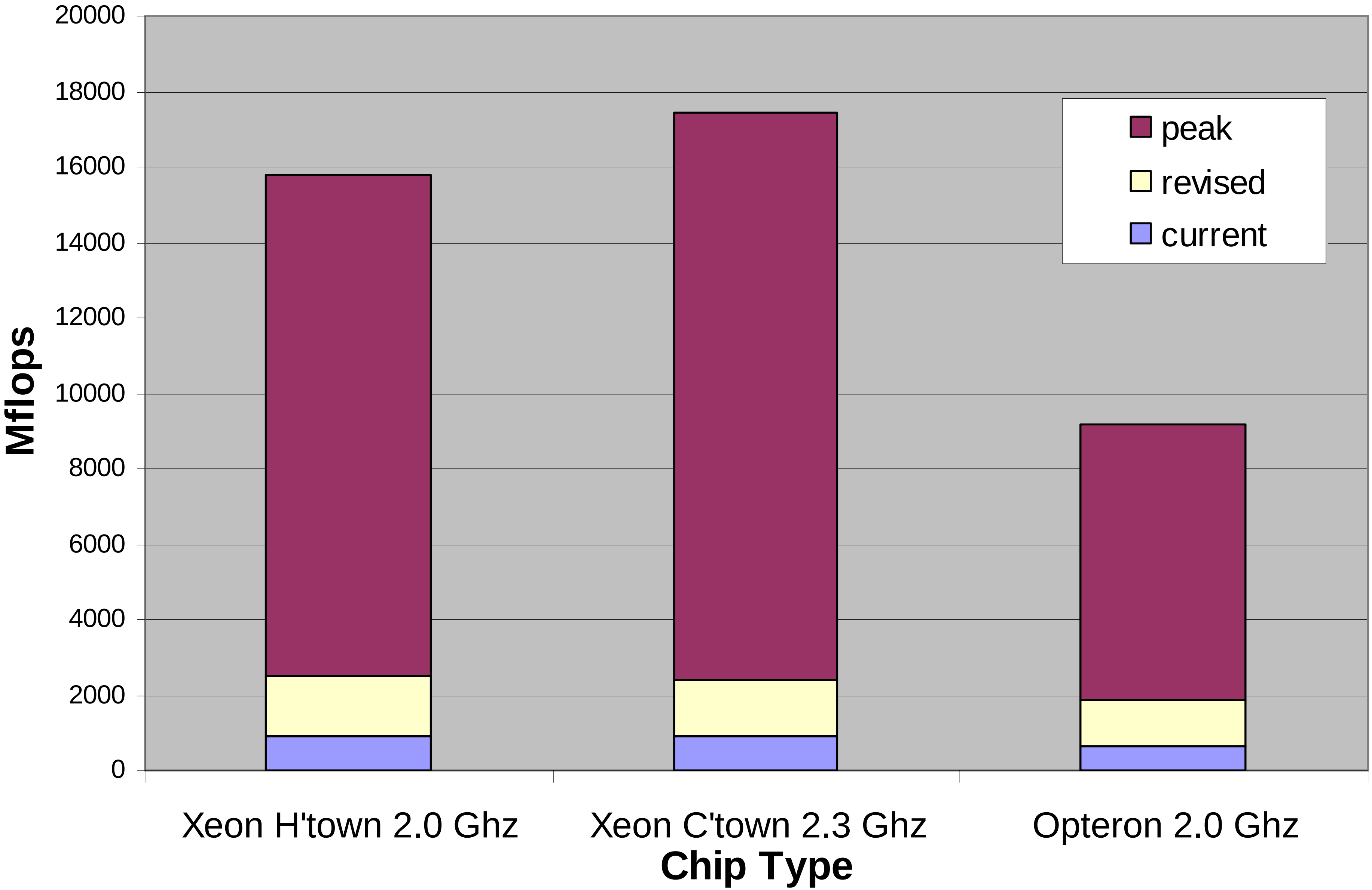
Benchmarks (Single Core, 2nd Order 72x72x53)



Benchmarks (Single Core, 2nd Order 24x24x24 - 1MB)



Benchmarks (Single Core, 4th Order 72x72x53)



Summary

- Notable improvement in % of peak from reduced memory footprint
- Longer vector lengths are better
- BUT: RK3 (revised) method still requires more wall clock time (>50%) for a single core, tests are underway to see if this is the case when using multiple cores
- Apply this method to the adv/mixing part of the existing code to improve performance (e.g. loop result)
- Recommendation: Apply higher order numerics to achieve higher % of peak (almost free)

Multi-Core Tests

- Compared current and revised (reduced memory requirement and revised order of computations) weather model
- MPI versions
- Timings for 1,2,4,8 cores per node on Sooner (OU Xeon-based Supercomputer)
- Sooner has two chips/node with 4 cores/chip
- Zero-slope line is perfect scaling

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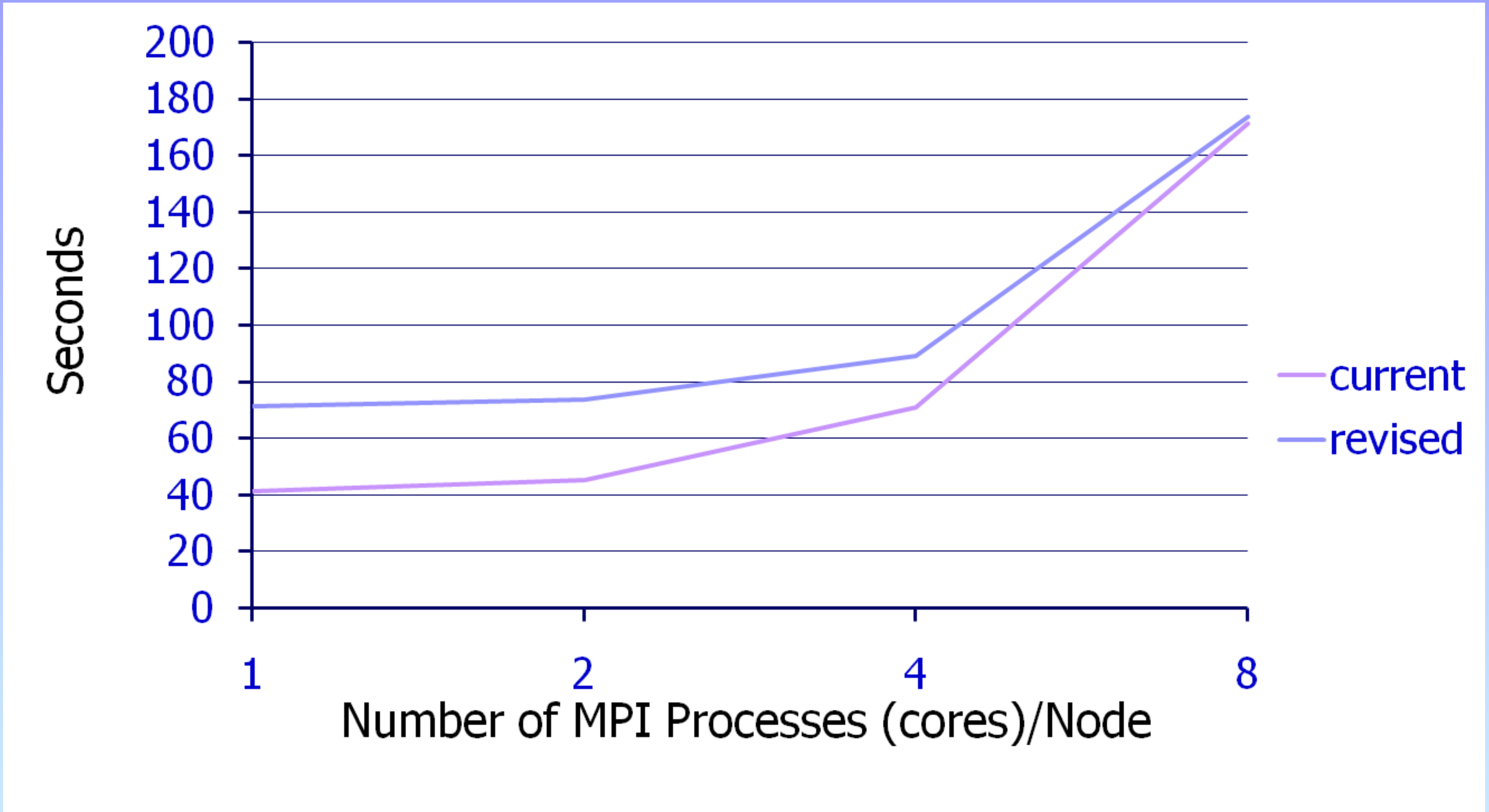
Multi-Core Benchmarks



Multi-Core Results Discussion

- Contention for the memory bus extends application run time
- 2 cores/node is approximately 90% efficient (2-10% overhead due to 2 cores accessing memory)
- 4 cores/node produces 25-75% overhead
- 8 cores/node produces 243-417% overhead (> 2-4 x slower than 1 processor test) – but doing 8x more work

Multi-Core Summary

- Multi-core performance scales very well at 2 cores/node but scalability is drastically reduced when using 8 cores/node
- Contention for memory becomes significant for memory intensive codes at 8 cores/node (OU Sooner HPC system)

- Credits:
  - Dr. Henry Neeman (OSCER)
  - Scott Hill (OU-CAPS PAPI)
  - PSC (David ONeal)
  - NCSA
  - Tinker AFB

Thank You!