NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Best Practices for Hybrid OpenMP/MPI Programming on Hopper. The Cray Center of Excellence: Performance Optimization for the Multicore Era GTC, Gamess, fvCAM and PARATEC

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The Multicore era

- Moore's Law continues
- Traditional sources of performance improvement ending
  - Old Trend: double clock frequency every 18th months
  - New Trend: Double # cores every 18 months
- Power Limits Drive a number of Broader Technology Trends
  - Number Cores ↑
  - Memory Capacity per core ↓
  - Memory Bandwidth per FLOP ↓
  - Network Bandwidth per FLOP ↓

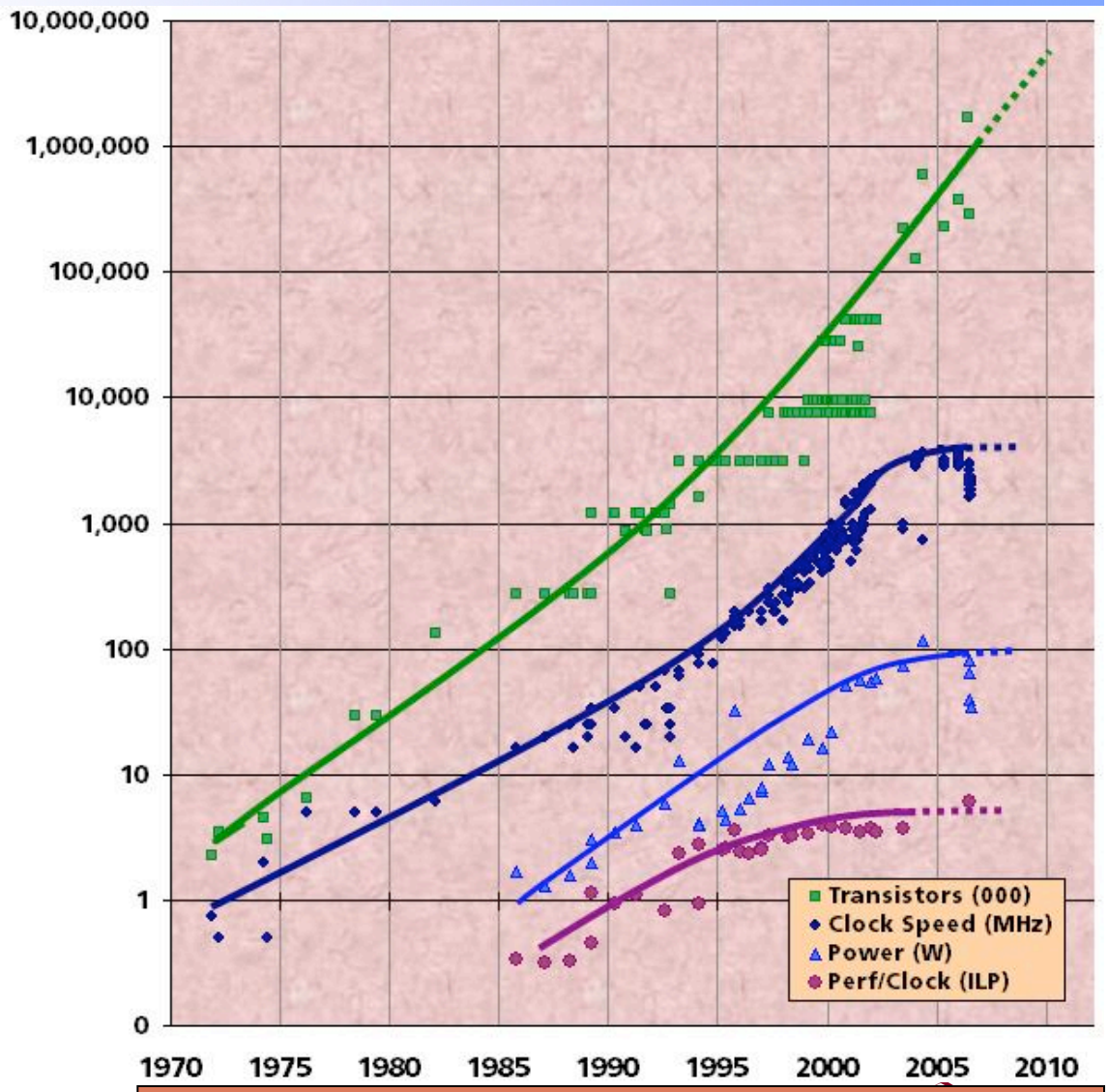

Figure courtesy of Kunle Olukotun, Lance Hammond, Herb Sutter, and Burton Smith

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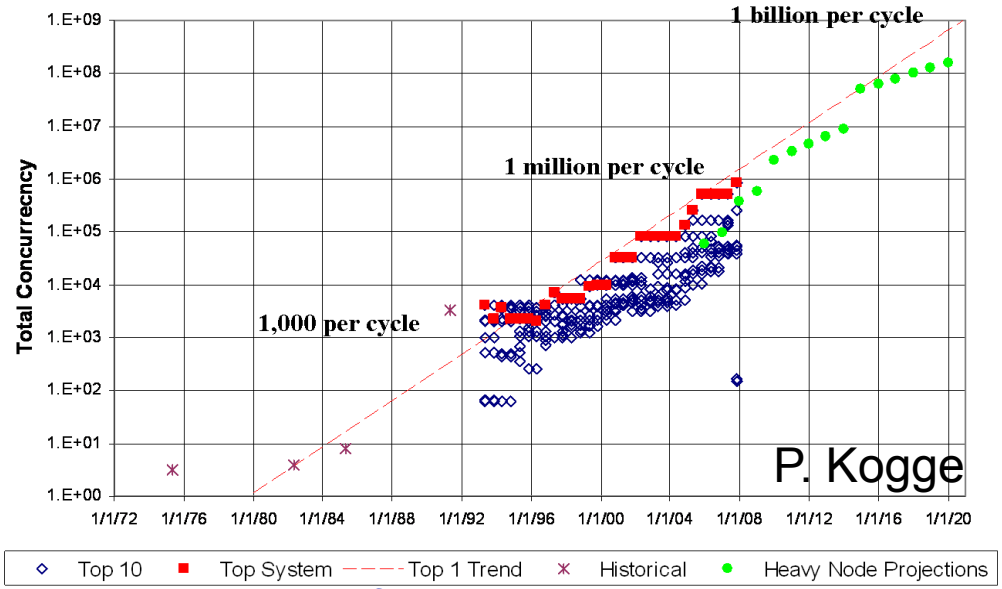
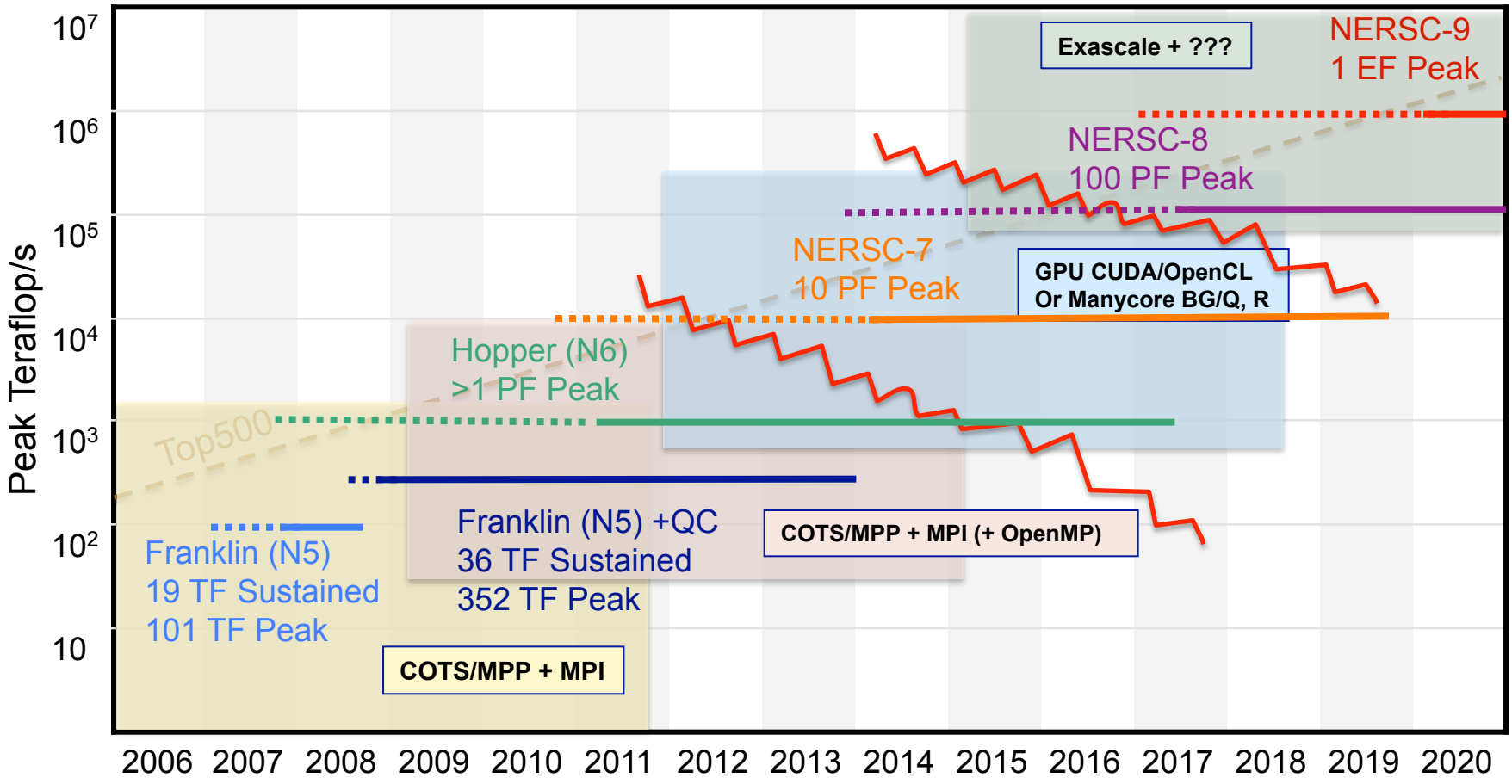


- **Implication for NERSC users**
  - **3x increase in system performance with no per-core performance improvement**
  - **12x more cores in NERSC-6 (hopper) than NERSC-5 (franklin) (4 cores to 24 cores)**
  - **Same or lower memory capacity per core on compute nodes**

- **Flat MPI-only model for parallelism will not scale**
  - **Need to transition to new model that can sustain massive growth in parallelism**
  - **Hopper changes are first step in a long-term technology trend**
  - **NERSC needs to take pro-active role in guiding transition of user community**

Long-Term Concerns for NERSC Users



Center of Excellence with Cray

Multicore Era: Massive on-chip concurrency necessary for reasonable power use

What should we tell NERSC users to do ?

NERSC/Cray "Programming Models Center of Excellence" combines:

- **Berkeley Lab strength in advanced programming models, multicore tuning, and application benchmarking**
- **Cray strength in advanced programming models, optimizing compilers, and benchmarking**

Immediate question: What is the best way to use cores in N6 (Hopper) node?

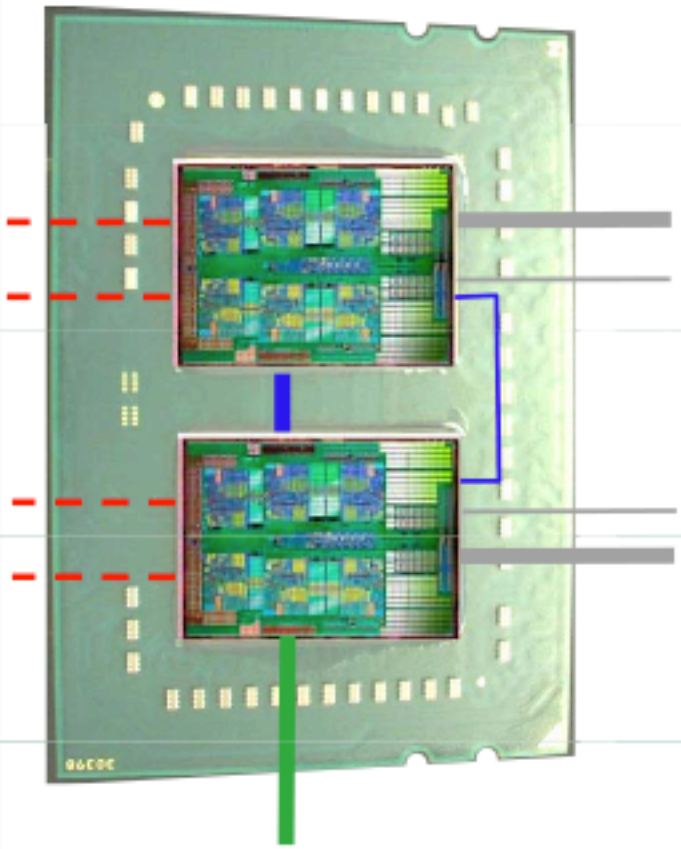
- **Flat MPI - Today's preferred mode of operation**
  - **Model has diverged from reality (the machine is NOT flat)**
  - **4 - 8 cores? ✔ 128 - 1024 cores? ✗**
- **MPI + OpenMP**
- **MPI + pthreads**
- **MPI + PGAS**
- **PGAS, CUDA, OPENCL, ….**

NERSC COE: Project Plan

- **Phase 1: Prepare users for Hopper**
  - NERSC-6 application benchmarks provide representative set of NERSC workload and broad cross-section of algorithms
  - User hybrid OpenMP/MPI model because it is most mature
  - Analyze performance of hybrid applications
  - Work with USG to create training materials for Hopper users

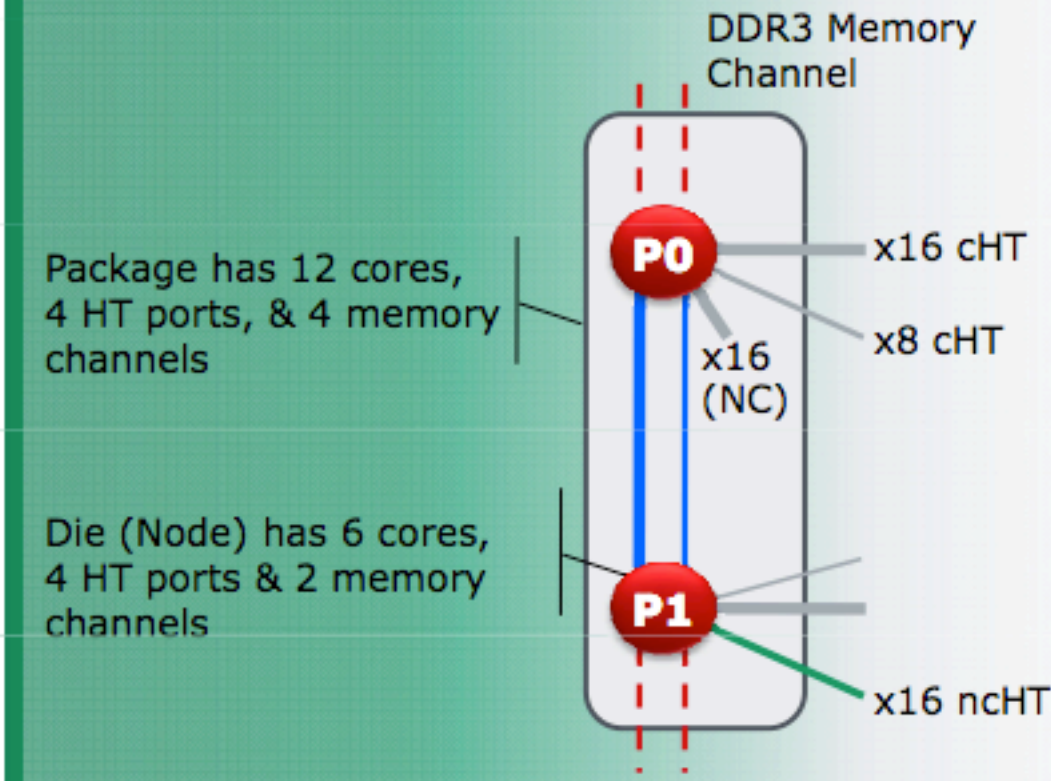
- **Phase 2: Prepare users for next decade**
  - Evaluate advanced programming models
  - Identify durable approach for programming on path to exascale

AMD – Magny-Cours



G34 Socket

"Magny-Cours" utilizes a ***Directly Connected*** MCM

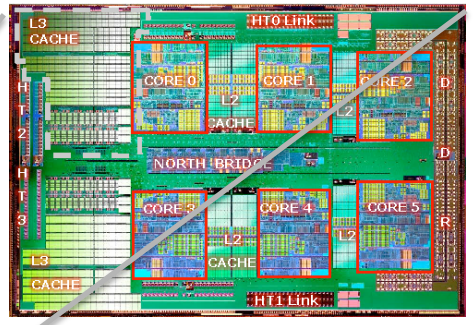


Package has 12 cores, 4 HT ports, & 4 memory channels

Die (Node) has 6 cores, 4 HT ports & 2 memory channels

Hopper Memory Heirarchy

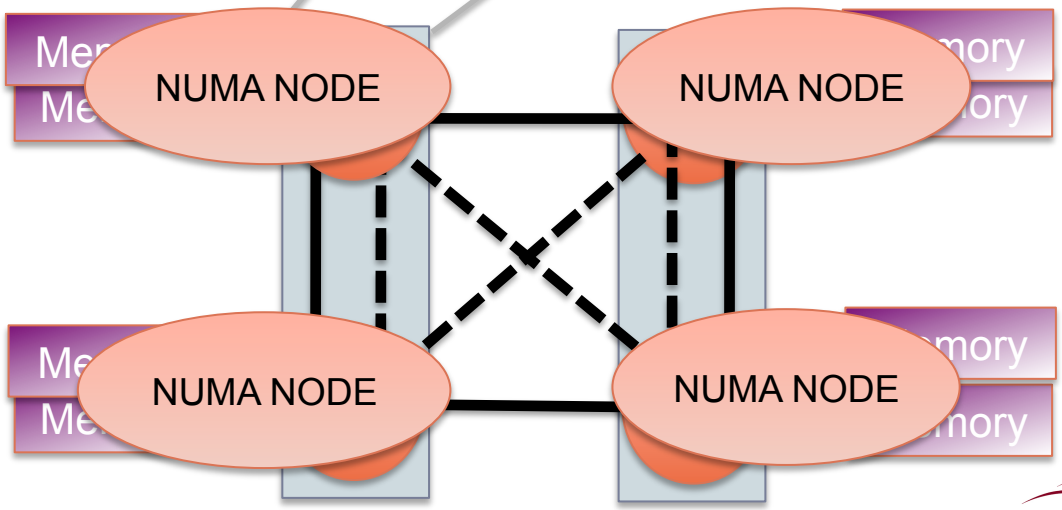
- "Deeper" Memory Hierarchy
  - NUMA: Non-Uniform Memory Architecture
  - All memory is transparently accessible but...
  - Longer memory access time to "remote" memory
  - A process running on NUMA node 0 accessing NUMA node 1 memory can adversely affect performance.



2xDDR1333 channel
21.3 GB/s

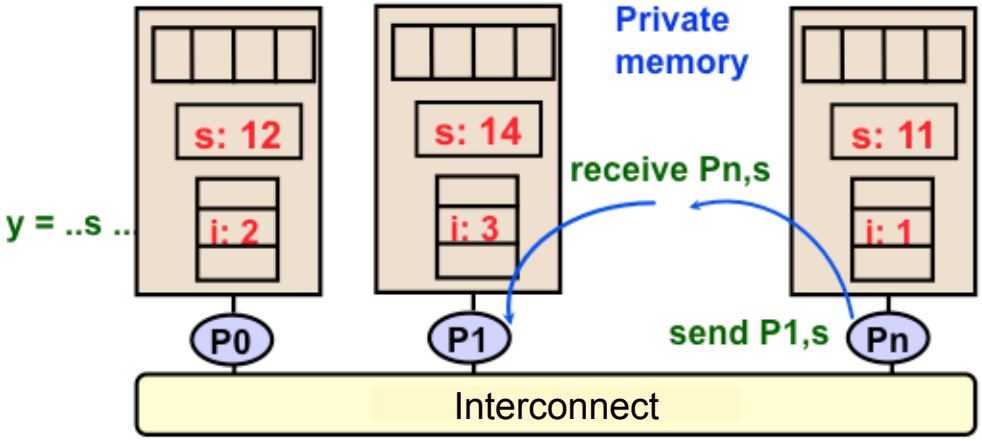
3.2GHz x16 lane HT
12.8 GB/s bidirectional

3.2GHz x8 lane HT
6.4 GB/s bidirectional



Hopper Node

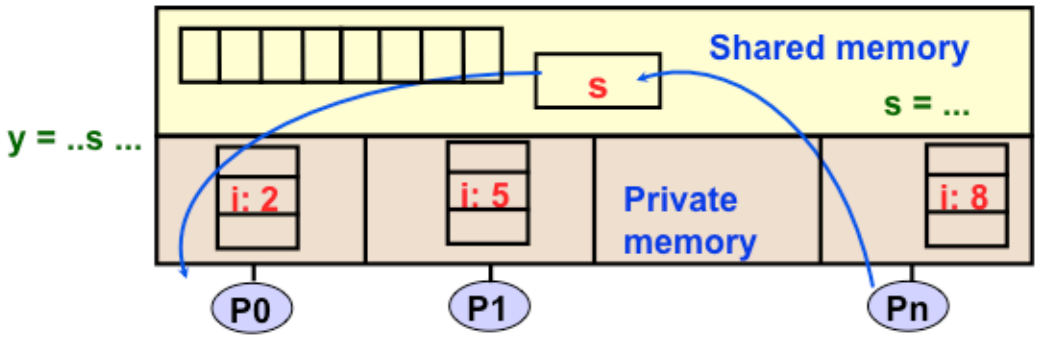
What are the Basic Differences Between MPI and OpenMP?



Message Passing Model

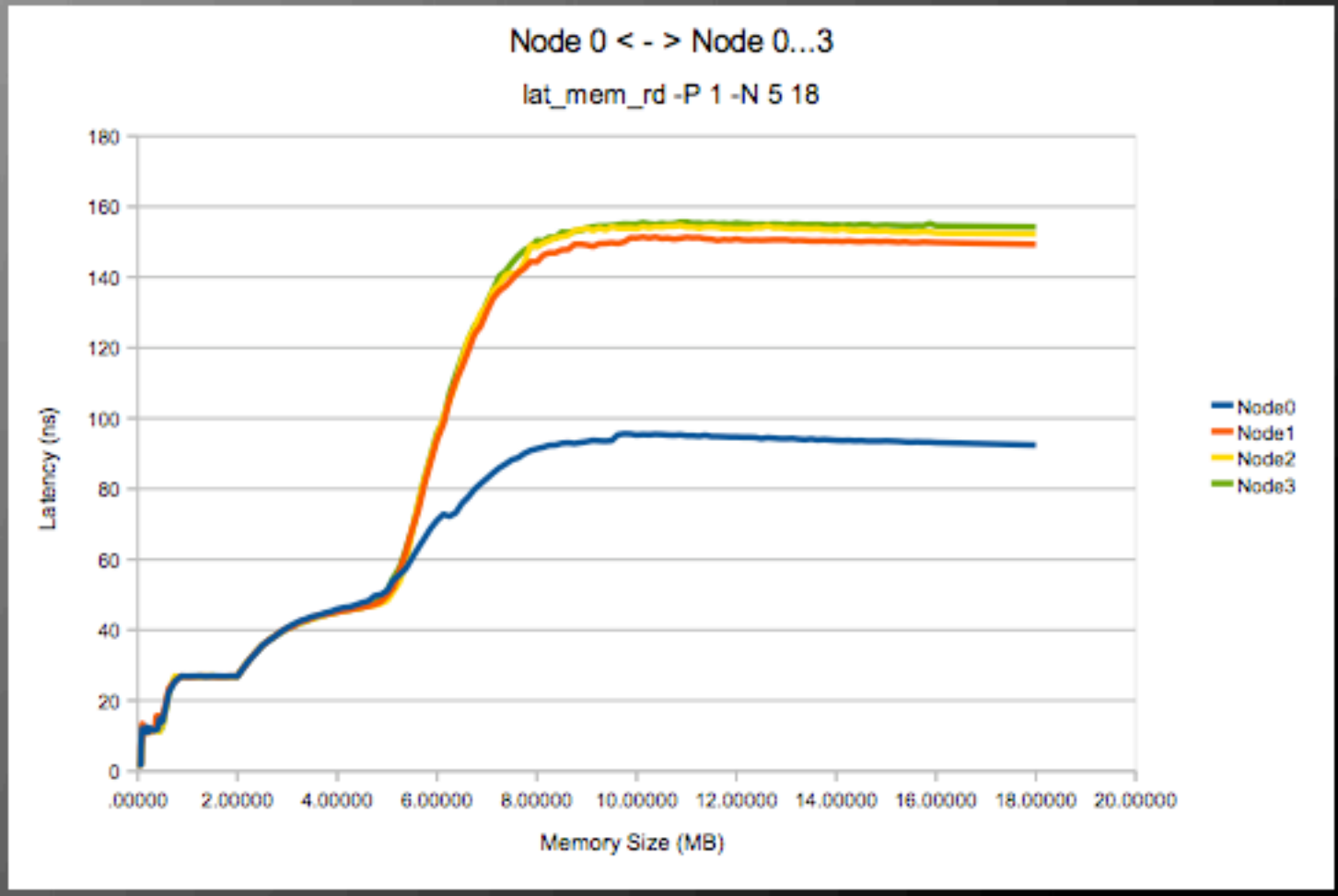
- Program is a collection of processes.
  - **Usually fixed at startup time**
- Single thread of control plus private address space -- NO shared data.
- Processes communicate by explicit send/ receive pairs
  - **Coordination is implicit in every communication event.**
- MPI is most important example.

Shared Address Space Model

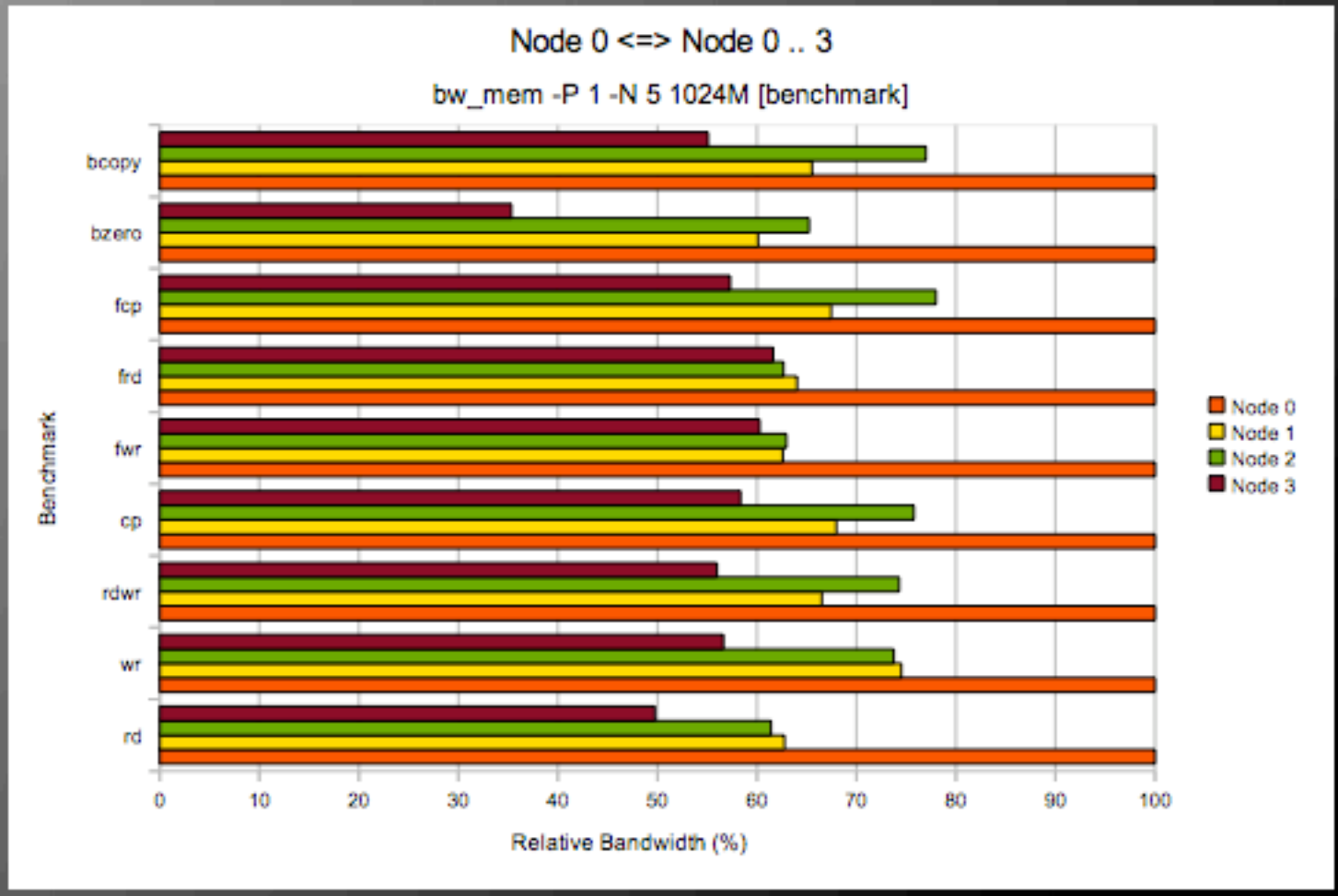


- Program is a collection of threads.
  - **Can be created dynamically.**
- Threads have private variables and shared variables
- Threads communicate implicitly by writing and reading shared variables.
  - **Threads coordinate by synchronizing on shared variables**
- OpenMP is an example

Why does it matter? - NUMA mem latency



Why does it matter? - NUMA mem bandwidth



Stream Benchmark

```
Double a[N],b[N],c[N};
.......
#pragma omp parallel for
#endif
    for (j=0; j<VectorSize; j++) {
      a[j] = 1.0; b[j] = 2.0; c[j] = 0.0;
    }
#pragma omp parallel for
 for (j=0; j<VectorSize; j++) {
      a[j]=b[j]+d*c[j];
}
```

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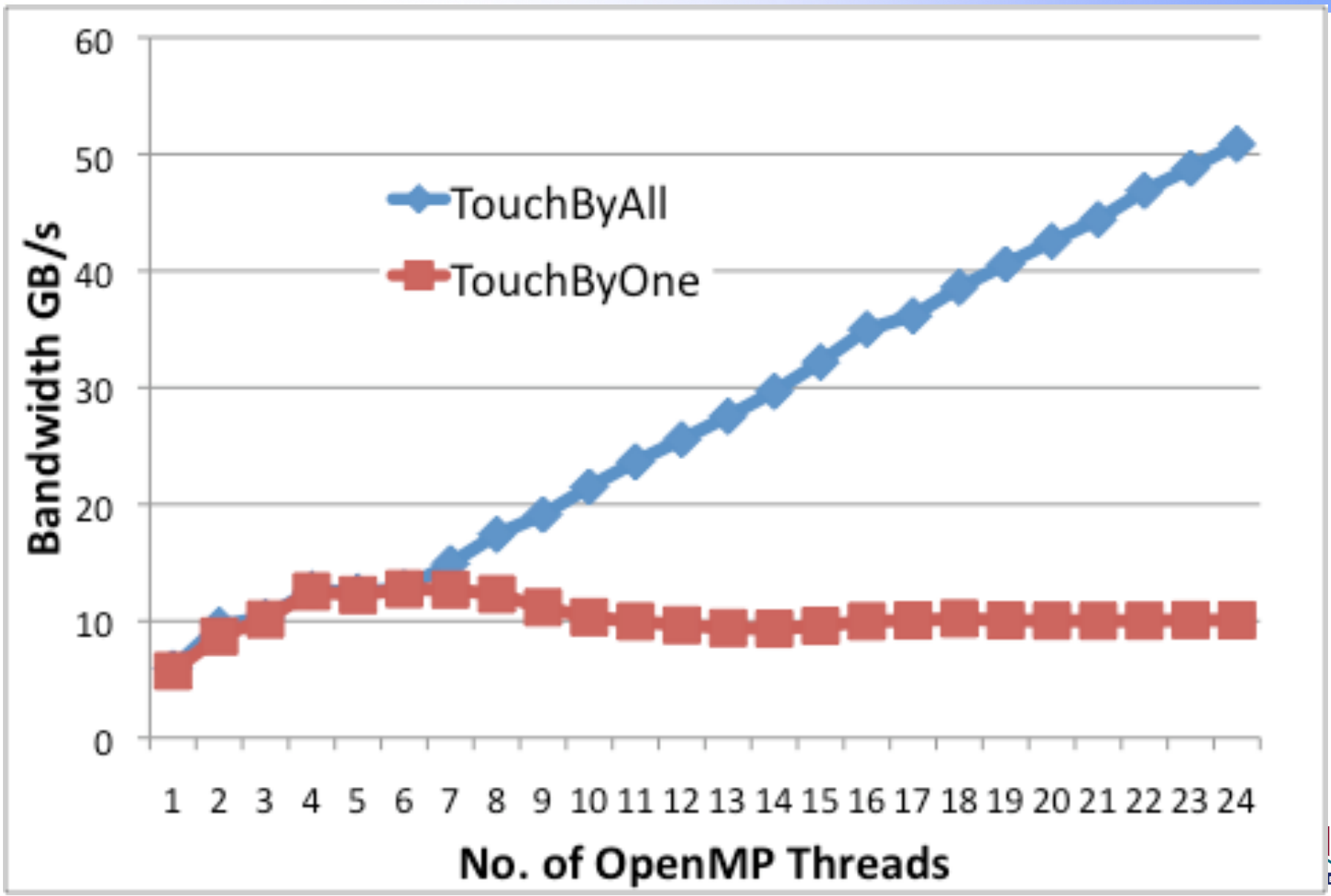
Stream NUMA effects - Hopper



NERSC-6 Applications Cover Algorithm and Science Space

Science areas	Dense linear algebra	Sparse linear algebra	Spectral Methods (FFT)s	Particle Methods	Structured Grids	Unstructured or AMR Grids
Accelerator Science		X	X IMPACT-T	X IMPACT-T	X IMPACT-T	X
Astrophysics	X	X MAESTRO	X	X	X MAESTRO	X MAESTRO
Chemistry	X GAMESS	X	X	X		
Climate			X CAM		X CAM	X
Combustion					X MAESTRO	X AMR Elliptic
Fusion	X	X		X GTC	X GTC	X
Lattice Gauge		X MILC	X MILC	X MILC	X MILC	
Material Science	X PARATEC		X PARATEC	X	X PARATEC	

Hybrid MPI-OpenMP Programming

Benefits

+ Less Memory usage
+ Focus on # nodes *(which is not increasing as fast)* instead of # cores
+ Larger messages, less time in MPI
+ Attack different levels of parallelism than possible with MPI

Potential Pitfalls

- NUMA / Locality effects
- Synchronization overhead
- Inability to saturate network adaptor

Mitigations

- User training
- Code examples using *real* applications
- Hopper system configuration changes
- Feedback to Cray on compiler & system software development

Important to Set Expectations

- OpenMP + MPI unlikely to be faster than pure MPI - but it will almost certainly use less memory
- Very important to consider your overall performance
  - individual kernels maybe slower with OpenMP but the code overall maybe faster
- Sometimes it maybe better to leave cores idle
  - #1 Memory Capacity
  - #2 Memory Bandwidth
  - #3 Network Bandwidth
  - #4 Flops…….

Understanding Hybrid MPI/OPENMP Model

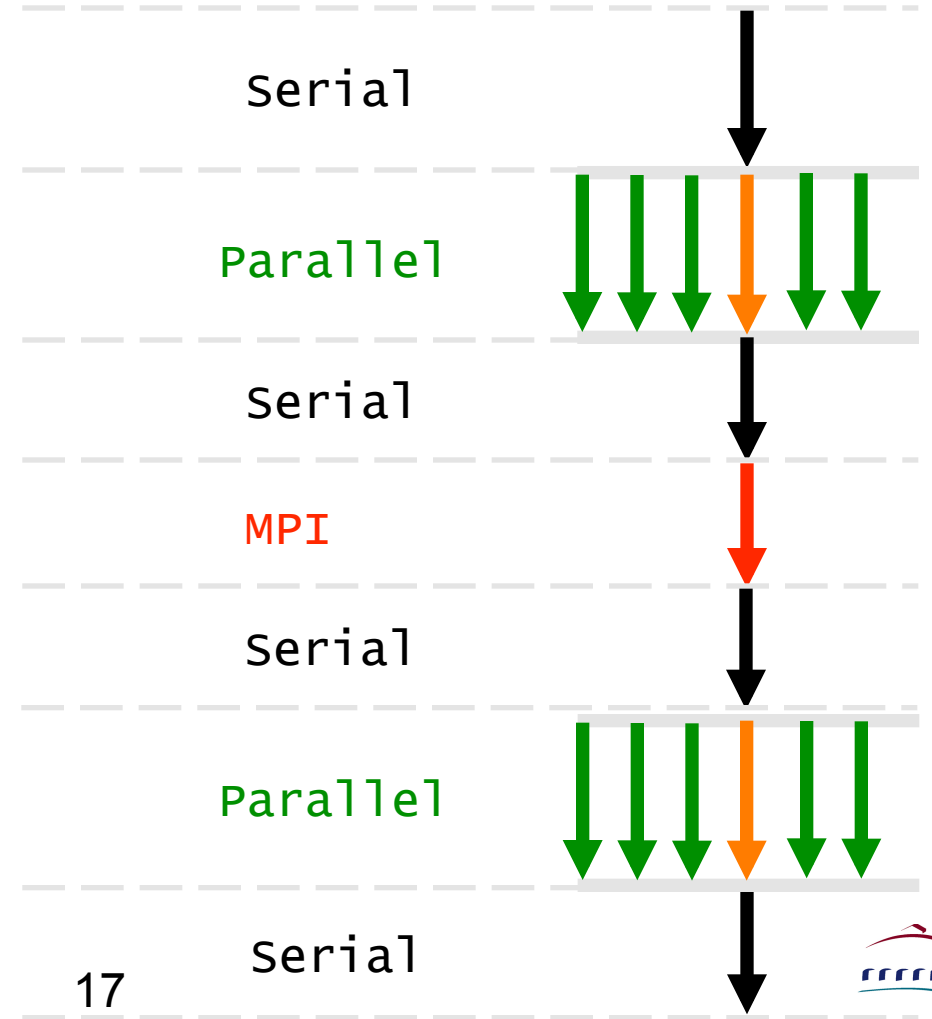
$T(N_{MPI},N_{OMP}) = t(N_{MPI}) + t(N_{OMP}) + t(N_{MPI},N_{OMP}) + t_{serial}$

```
count=G/N_MPI
  Do i=1,count
```

```
count=G/N_OMP
!$omp do private (i)
Do i=1,G
```

```
count=G/(N_OMP*N_MPI)
!$omp do private (i)
Do i=1,G/N_MPI
```

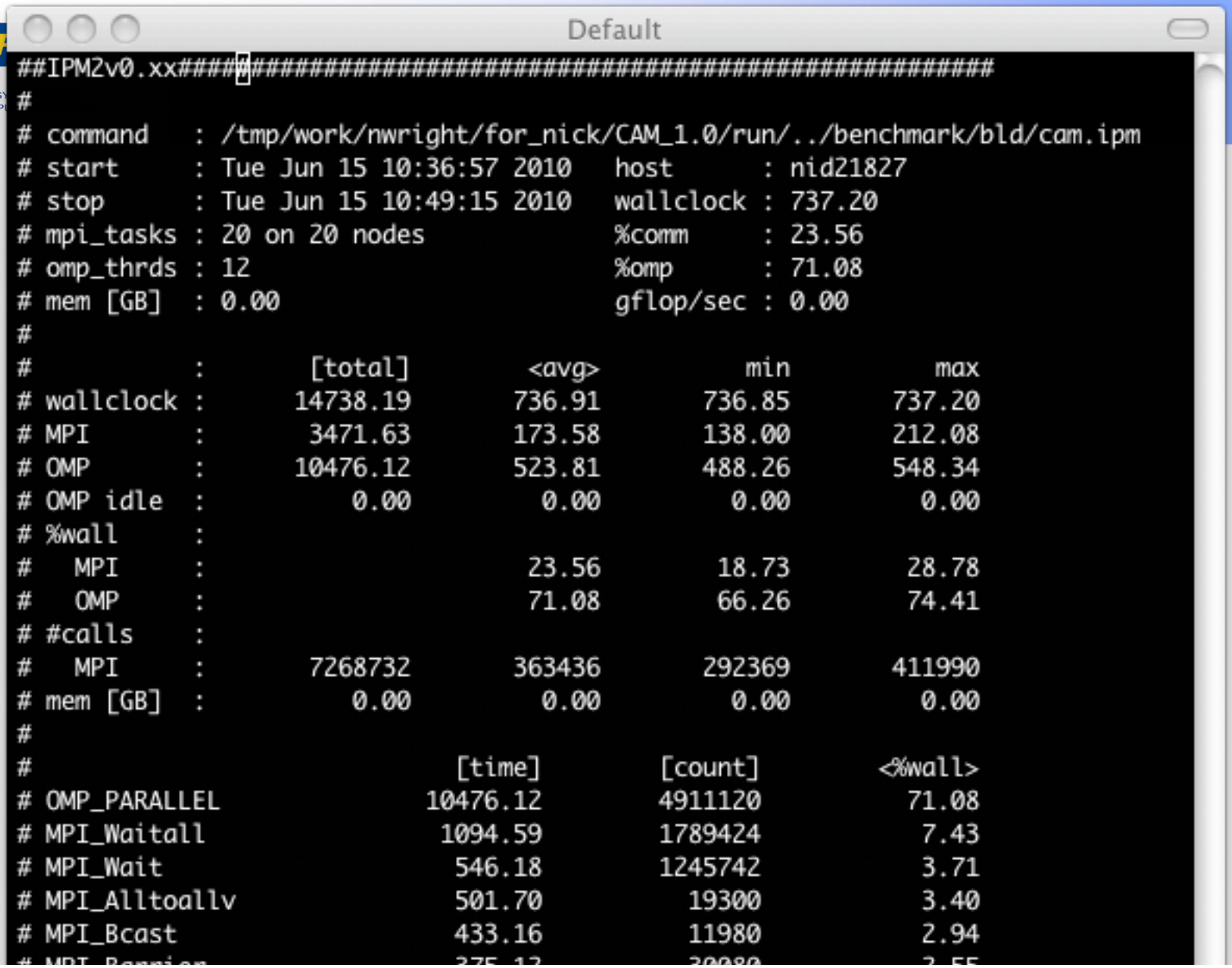
```
count=G
Do i=1,G
```



Breaking Down the Runtime - Tools

- **IPM – Integrated Performance Monitoring**
  http://ipm-hpc.sourceforge.net
  - **Time in MPI, Messages sizes, Communication Patterns**
  - **Simple Interface to PAPI**
  - **OpenMP profiler module added**
- **OMPP – OpenMP Profiler**

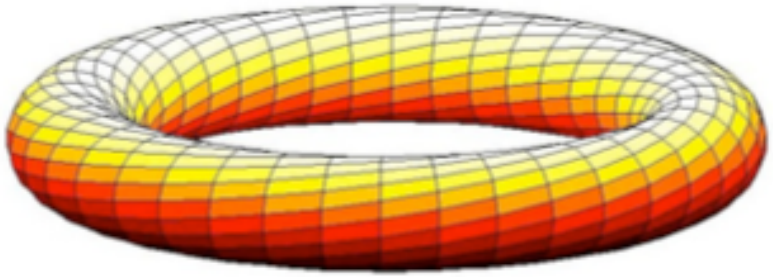
  http://www.cs.utk.edu/~karl/ompp.html
  - **Time Spent in Openmp per region, Load imbalance, Overhead**
  - **Also Interfaces to PAPI**


Default
##IPM2v0.xx##
#
command : /tmp/work/nwright/for_nick/CAM_1.0/run/../benchmark/bld/cam.ipm
start : Tue Jun 15 10:36:57 2010 host : nid21827
stop : Tue Jun 15 10:49:15 2010 wallclock : 737.20
mpi_tasks : 20 on 20 nodes %comm : 23.56
omp_thrds : 12 %omp : 71.08
mem [GB] : 0.00 gflop/sec : 0.00
#
: [total] <avg> min max
wallclock : 14738.19 736.91 736.85 737.20
MPI : 3471.63 173.58 138.00 212.08
OMP : 10476.12 523.81 488.26 548.34
OMP idle : 0.00 0.00 0.00 0.00
%wall :
MPI : 23.56 18.73 28.78
OMP : 71.08 66.26 74.41
#calls :
MPI : 7268732 363436 292369 411990
mem [GB] : 0.00 0.00 0.00 0.00
#
[time] [count] <%wall>
OMP_PARALLEL 10476.12 4911120 71.08
MPI_Waitall 1094.59 1789424 7.43
MPI_Wait 546.18 1245742 3.71
MPI_Alltoallv 501.70 19300 3.40
MPI_Bcast 433.16 11980 2.94

Talk Outline

- Gyrokinetic Toroidal Code (GTC)
- Parallel Total Energy Code (PARATEC)
- Finite Volume Community Atmosphere Model (fvCAM)
- General Atomic and Molecular Electronic Structure System (Gamess)
- Conclusions
- Next Steps

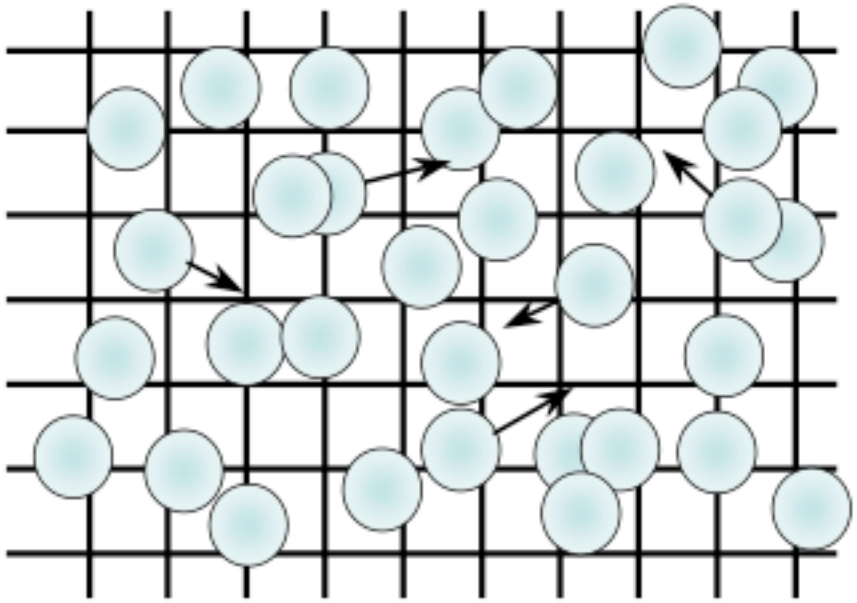
Gyrokinetic Toroidal Code (GTC)



- 3D Particle-in-cell (PIC)
- Used for simulations of non-linear gyrokinetic plasma microturbulence
- Paralleised with OpenMP and MPI.
- ~15K lines of Fortran 90
- OpenMP version 56 parallel regions/loops (almost all)
- 10 loops required different implementation for OpenMP version (~250 lines)

Particle-in-cell (PIC) method

- Particles sample distribution function (markers).
- The particles interact via a grid, on which the potential is calculated from deposited charges.

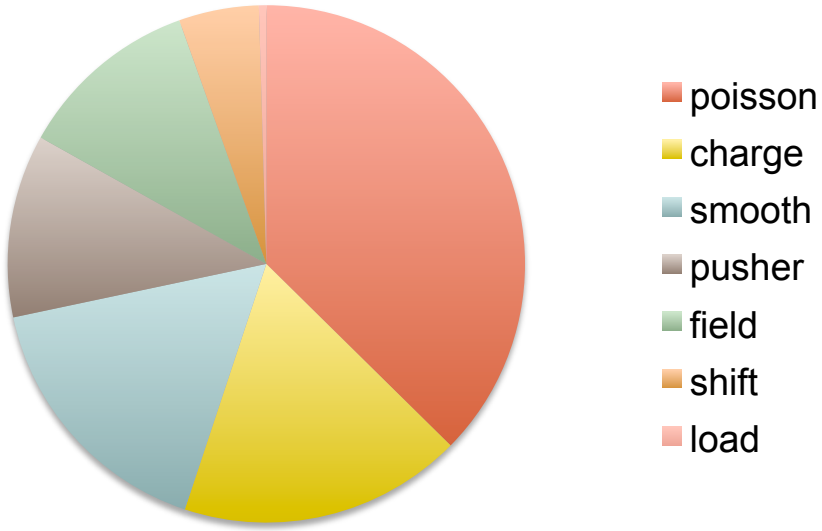


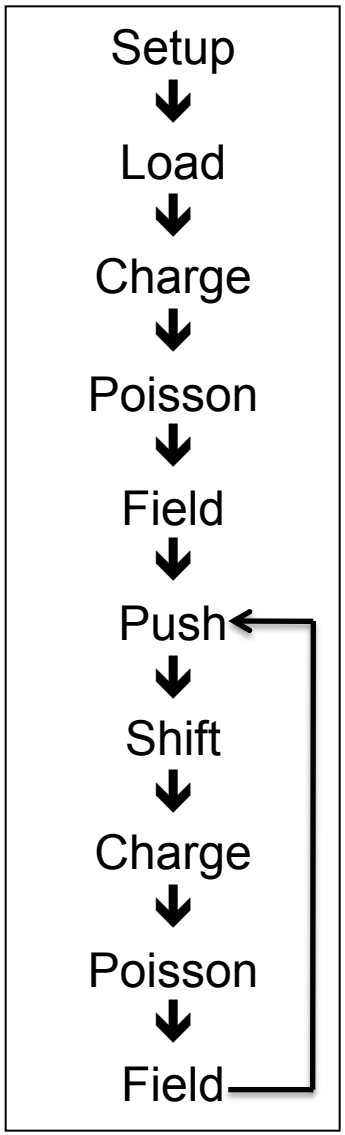
The PIC Steps

- "SCATTER", or deposit, charges on the grid (nearest neighbors)
- Solve Poisson equation
- "GATHER" forces on each particle from potential
- Move particles (PUSH)
- Repeat…

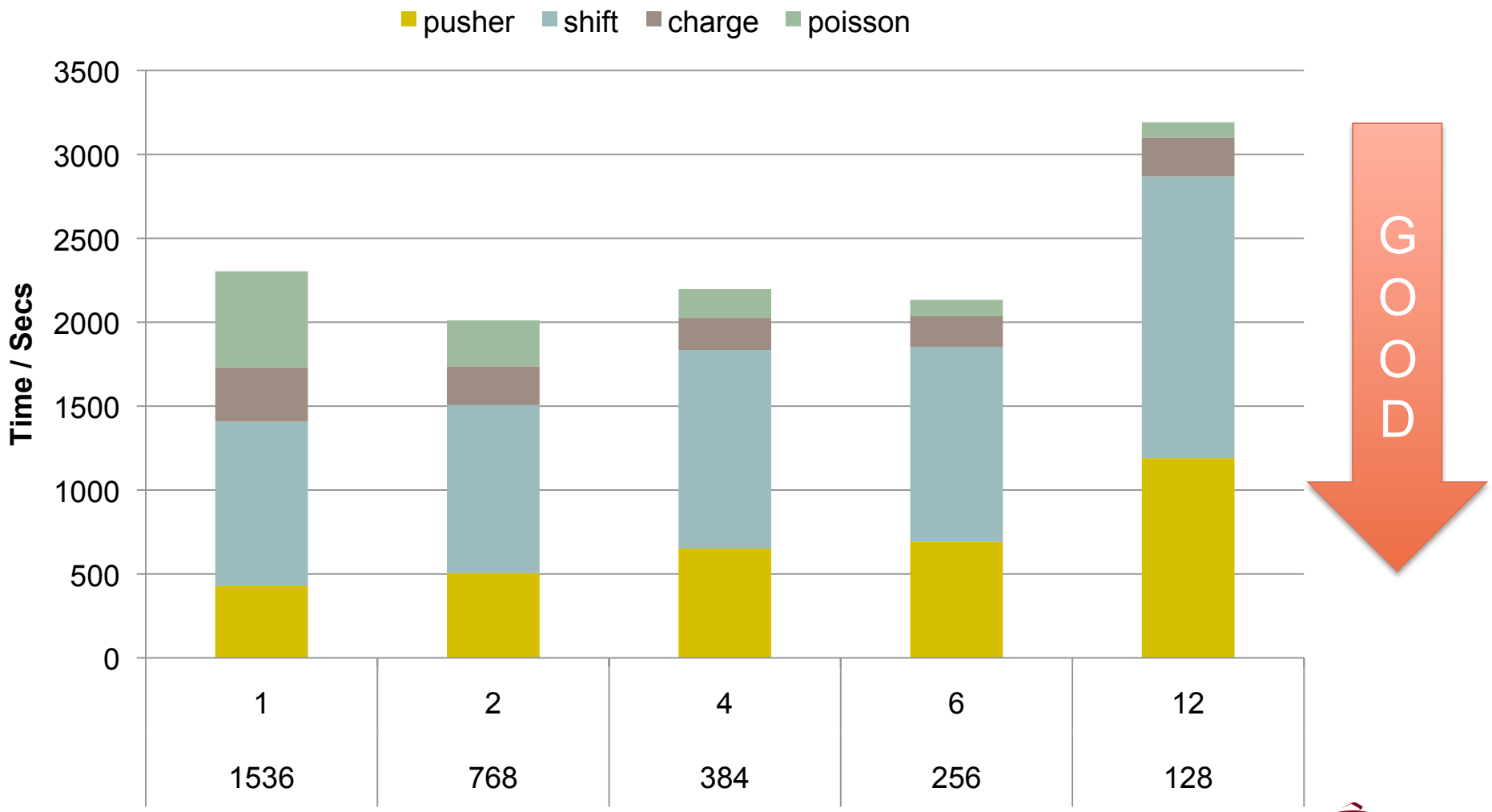
Important Routines in GTC

Poisson – charge distribution ➔ Electric field
Charge – deposits charge on Grid
Smooth – smoothes charge on grid
Pusher – Moves the Ions/Electrons
Field – Calculates Forces due to Electric field
Shifter – Exchanges between MPI tasks

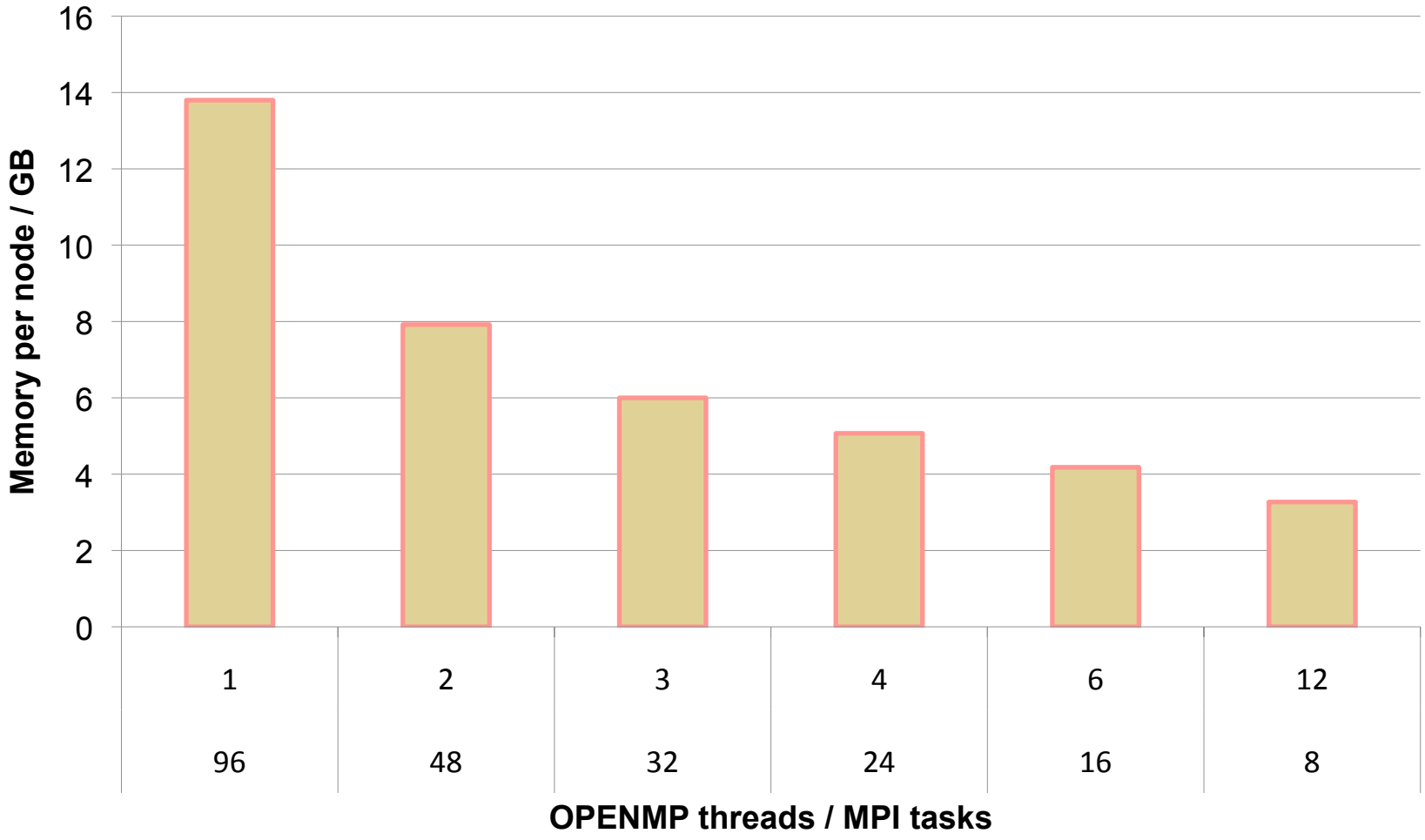




GTC MPI+OpenMP Performance



GTC - Memory Usage



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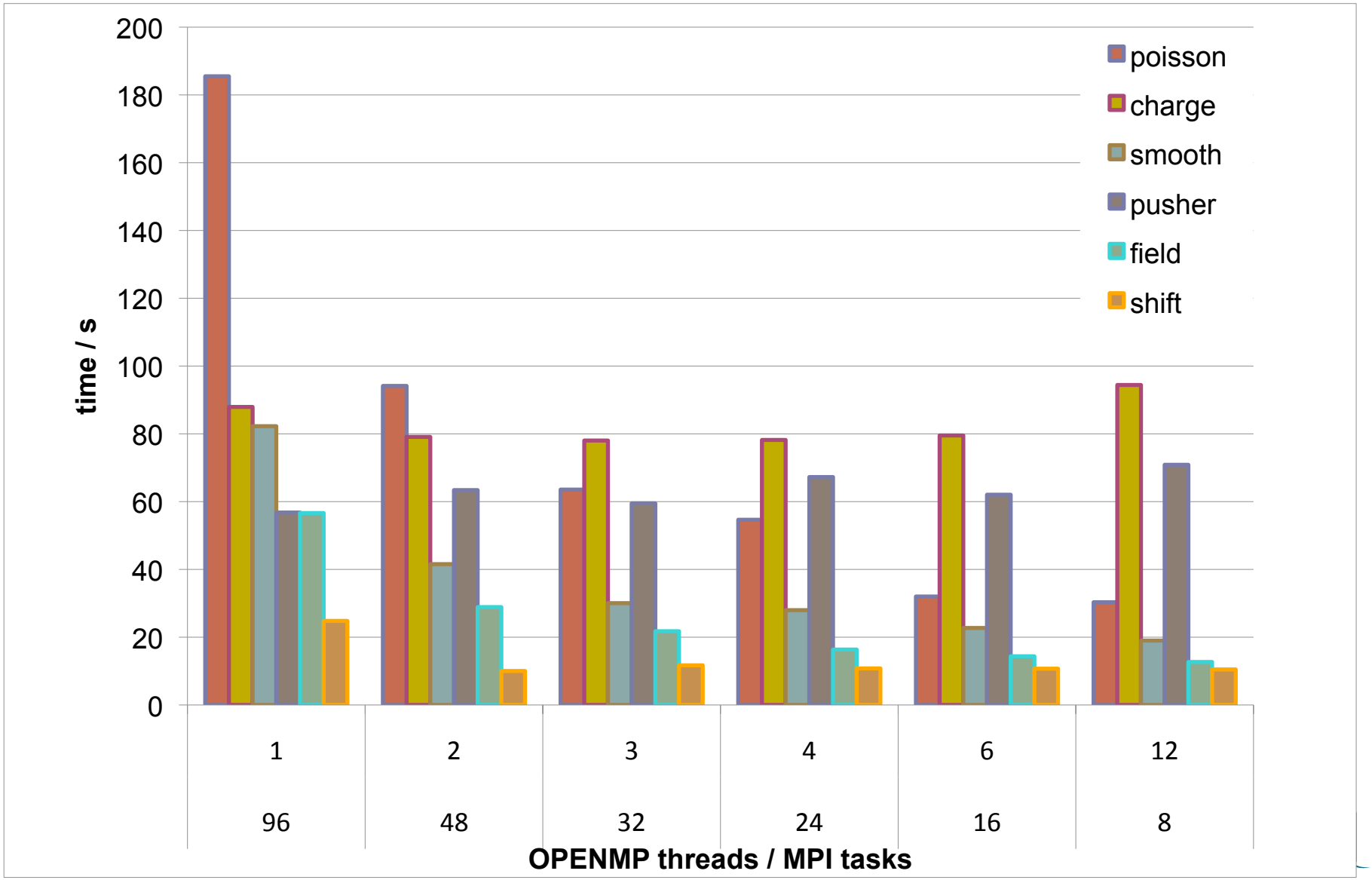
Small Test Case – 96 cores – Breakdown



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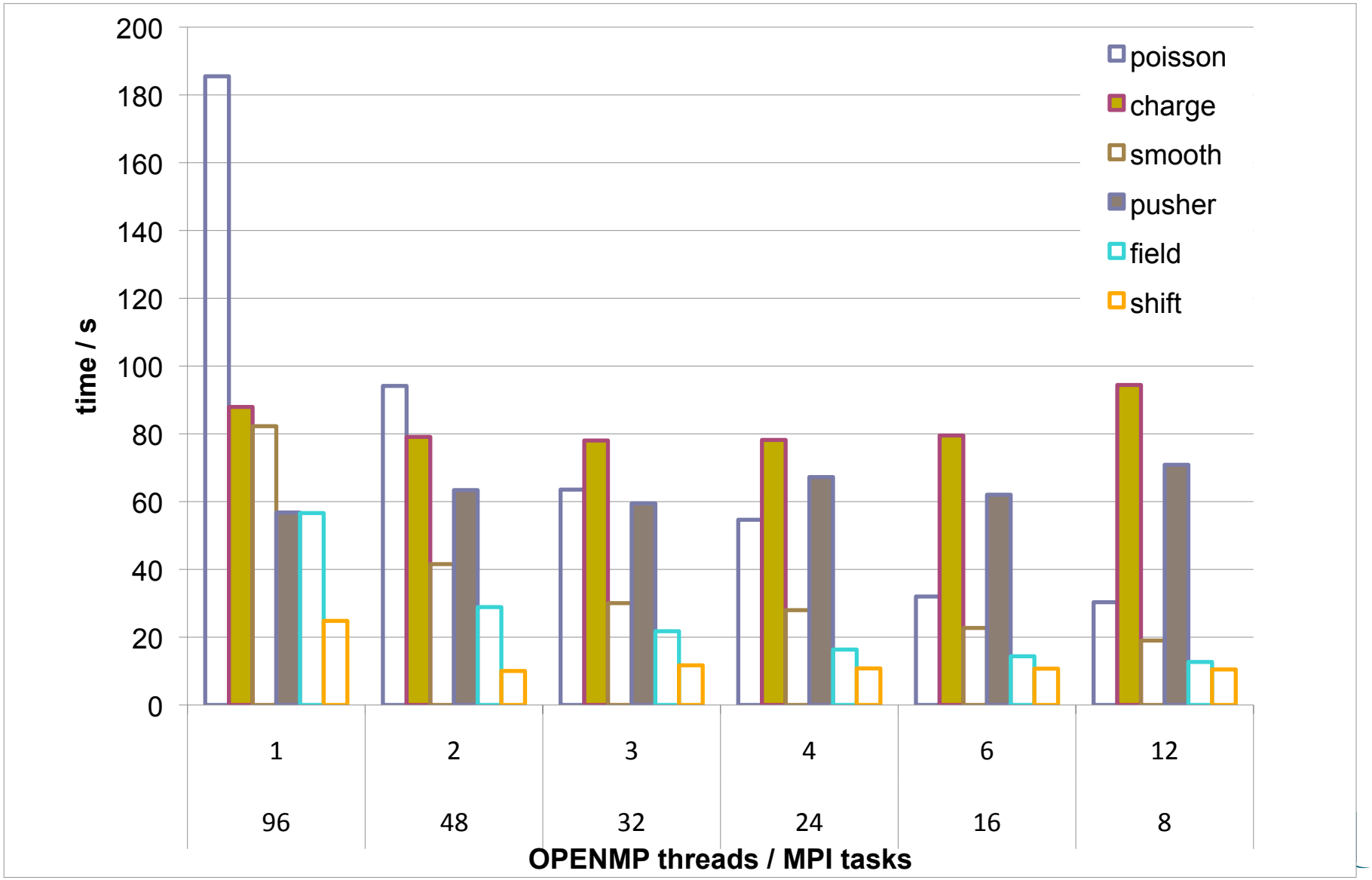

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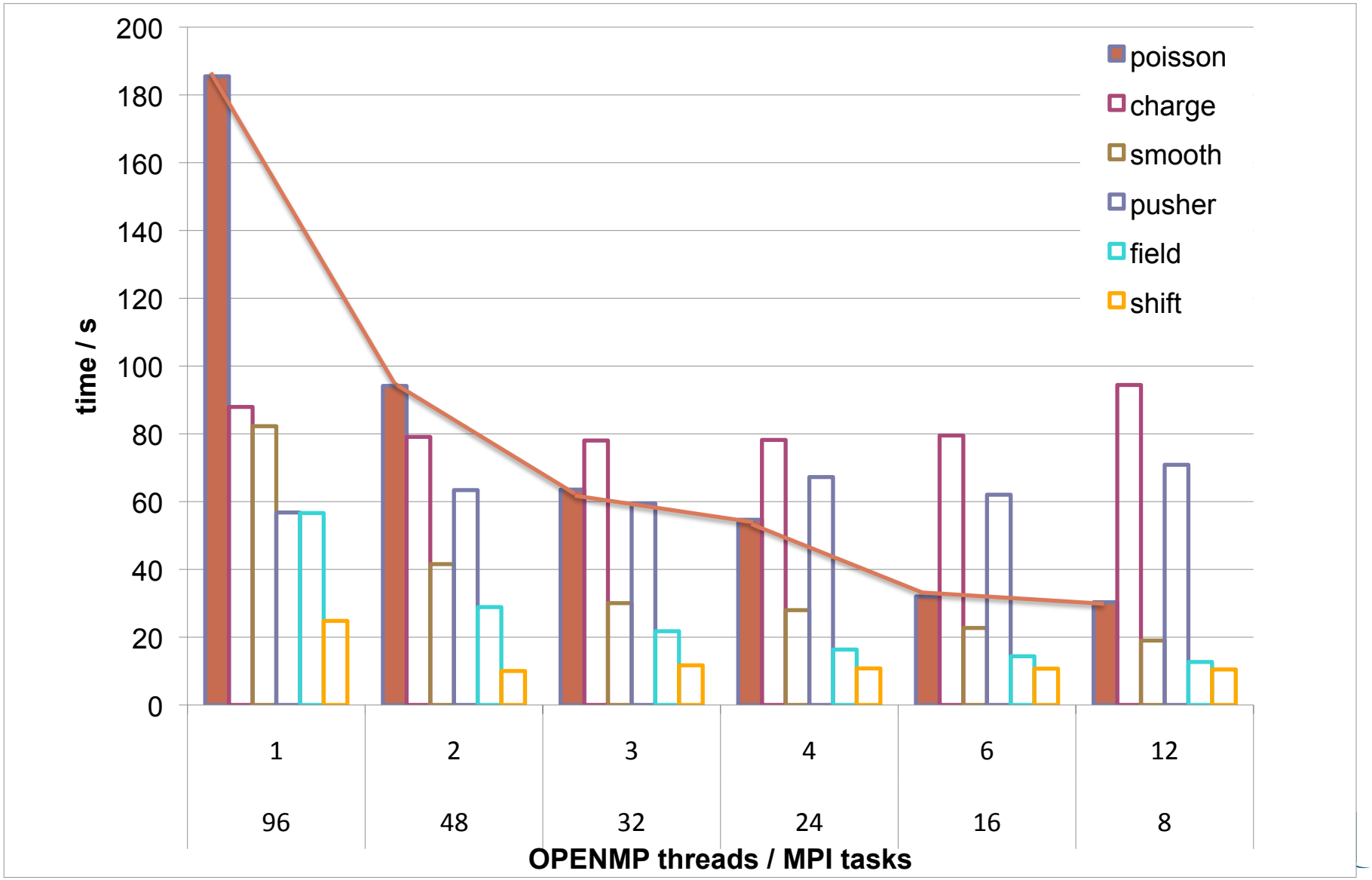
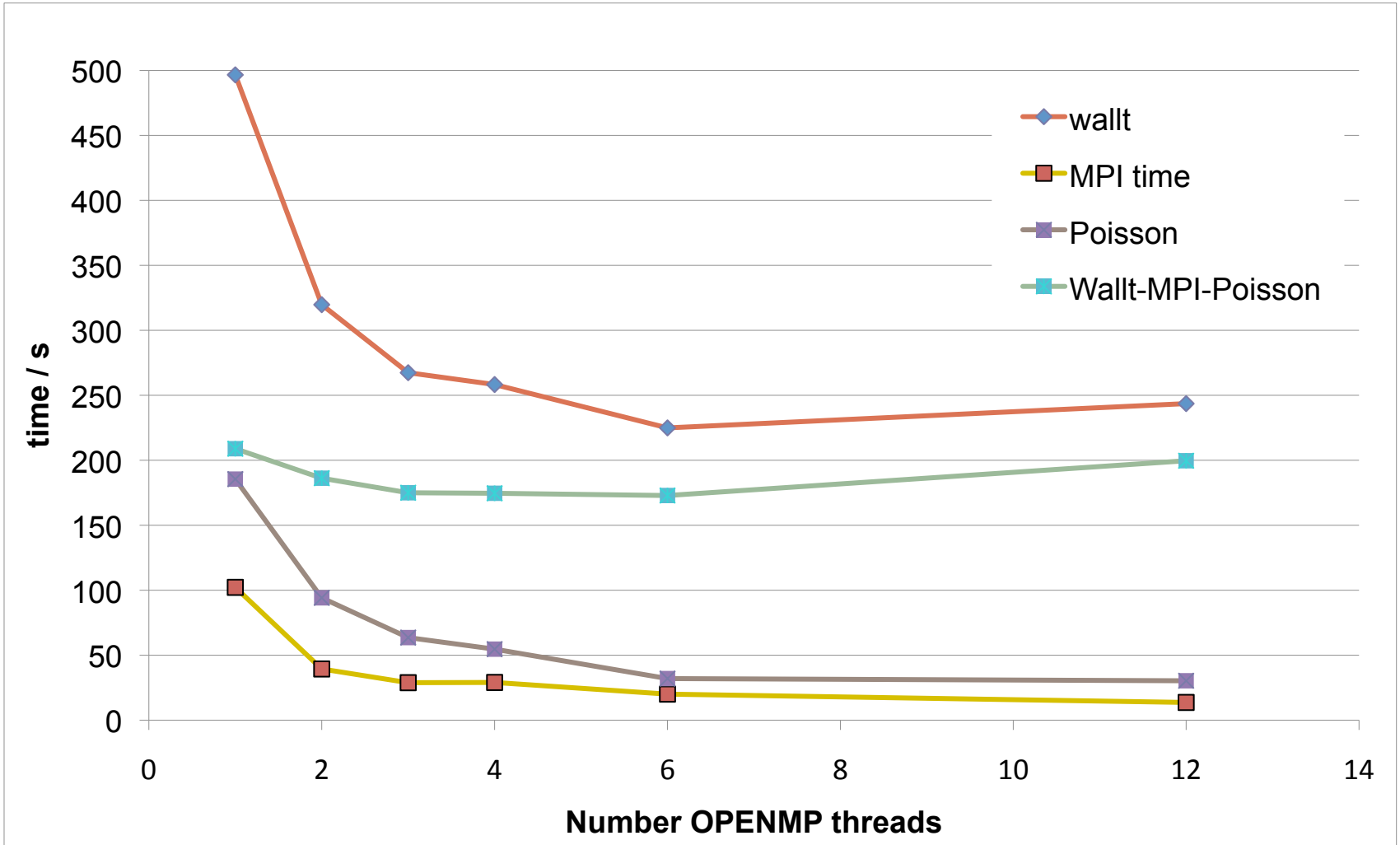
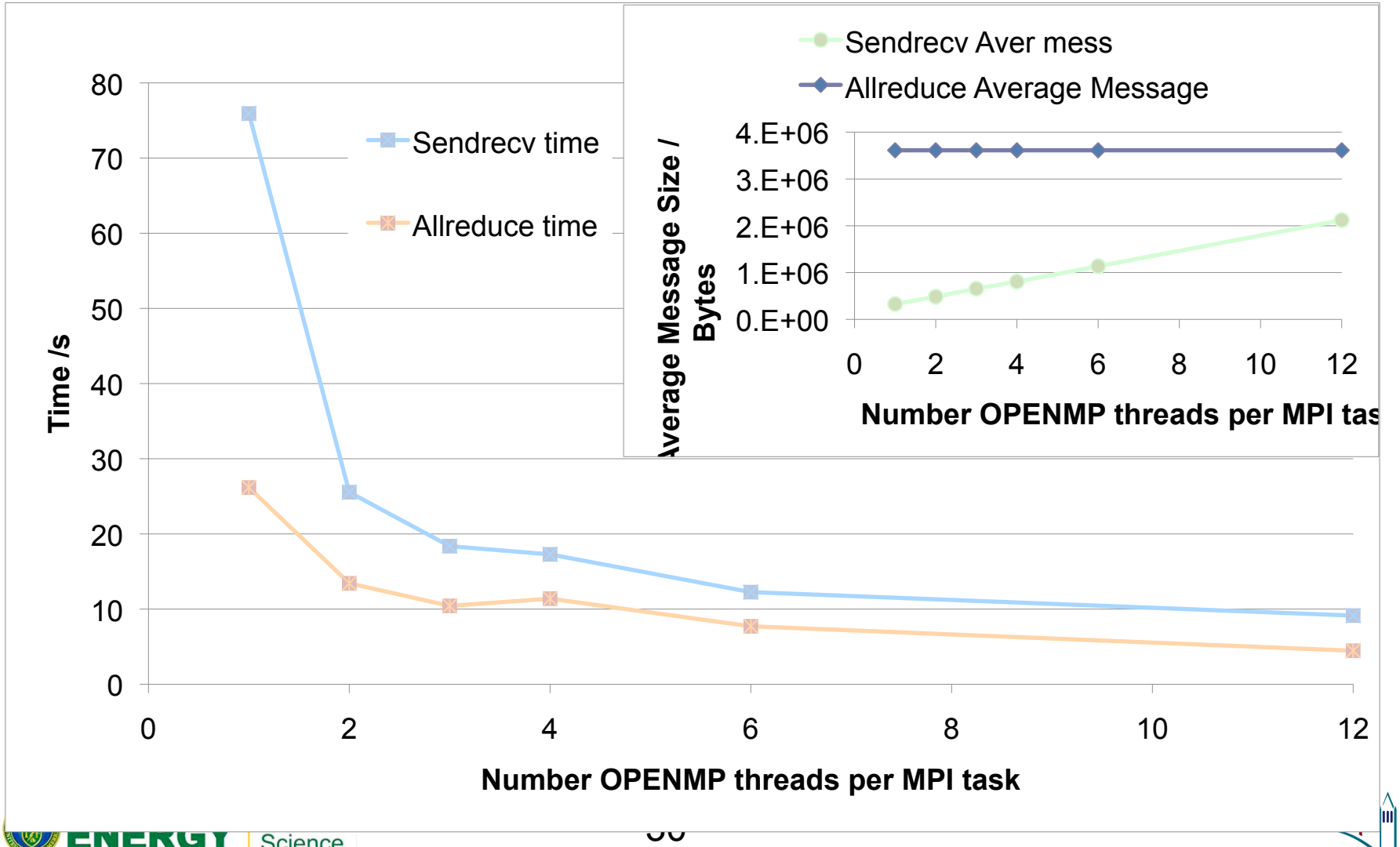


Small Case - Performance Breakdown



GTC: Communication Analysis



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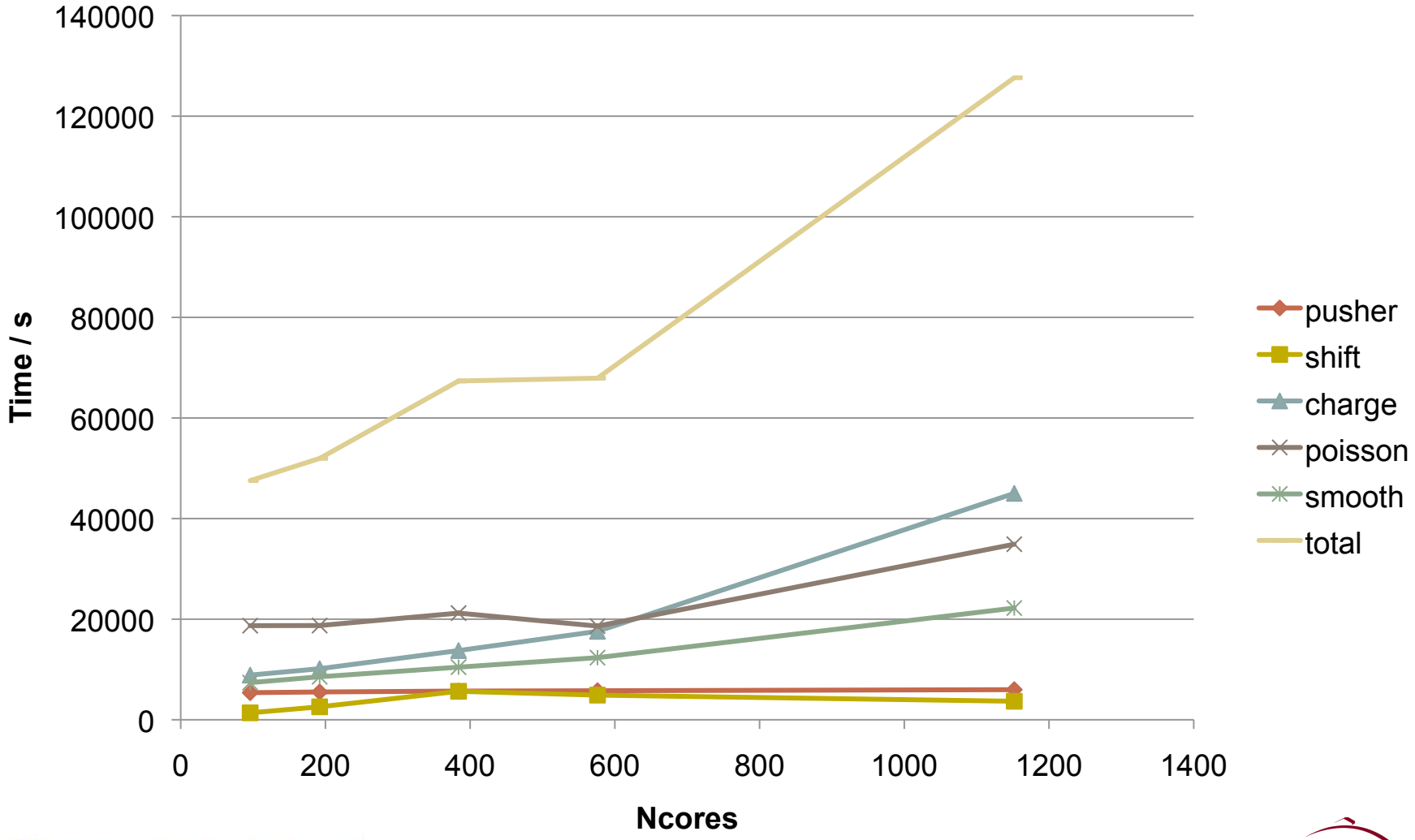
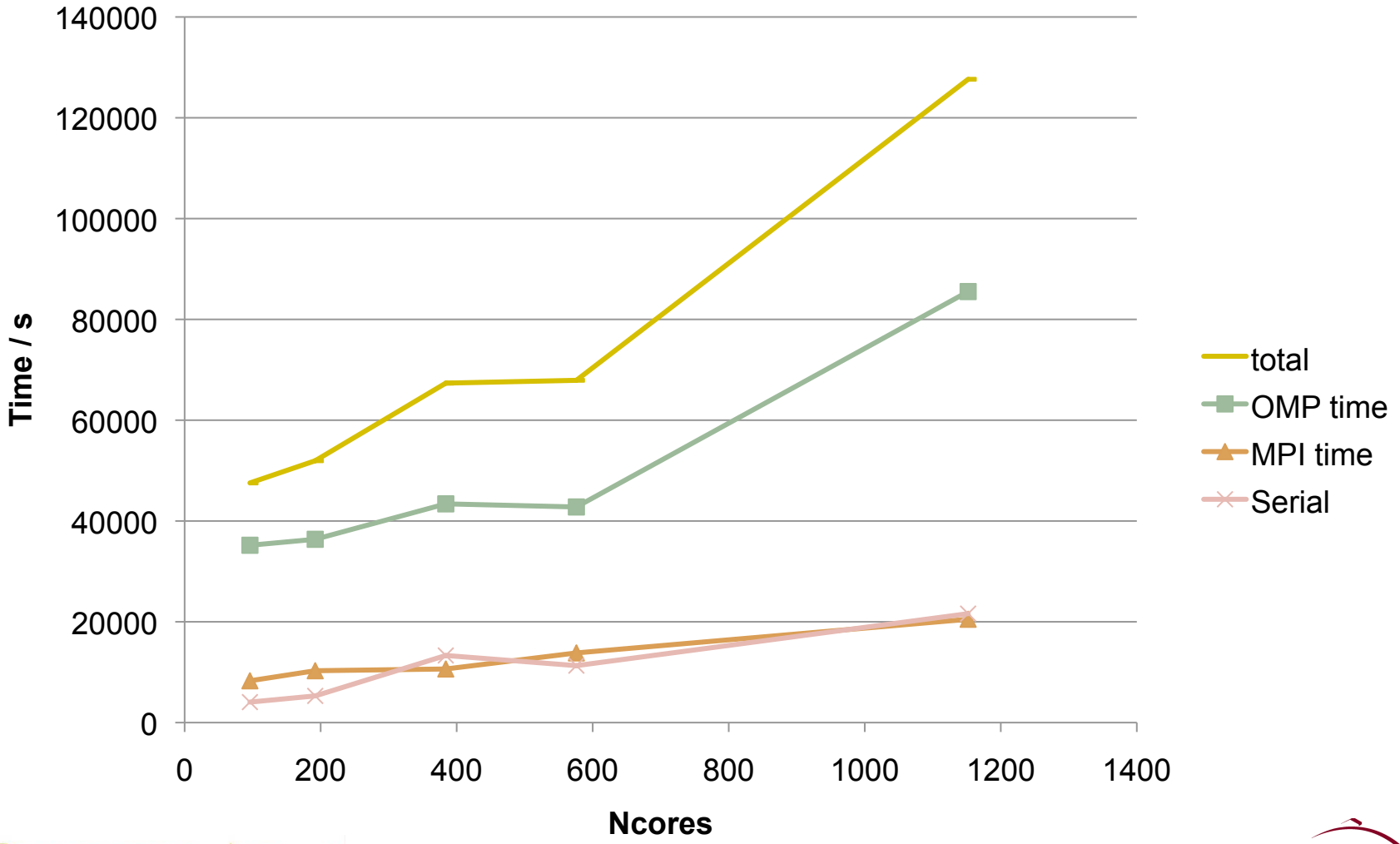
Strong Scaling

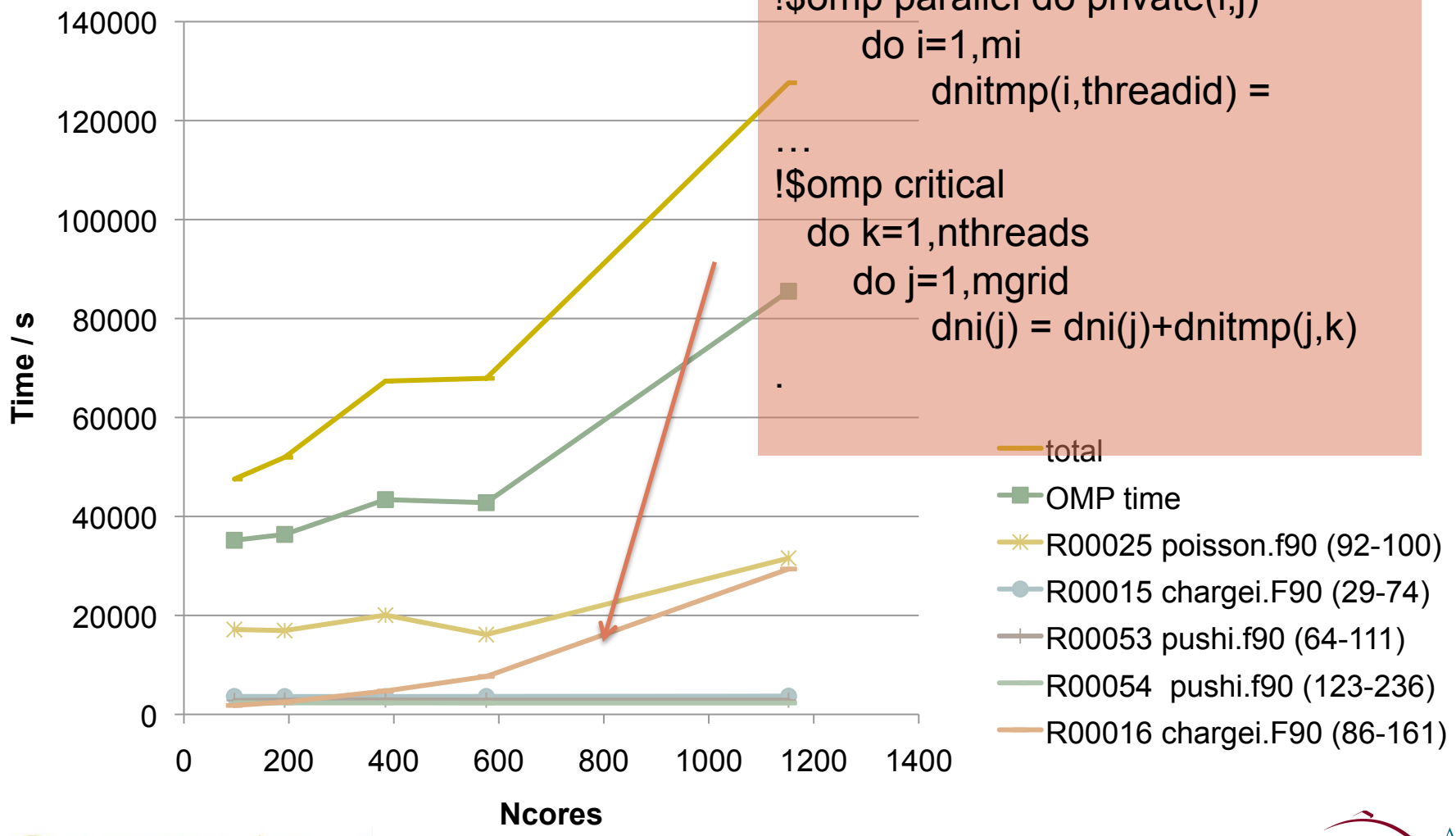


Strong Scaling cont.



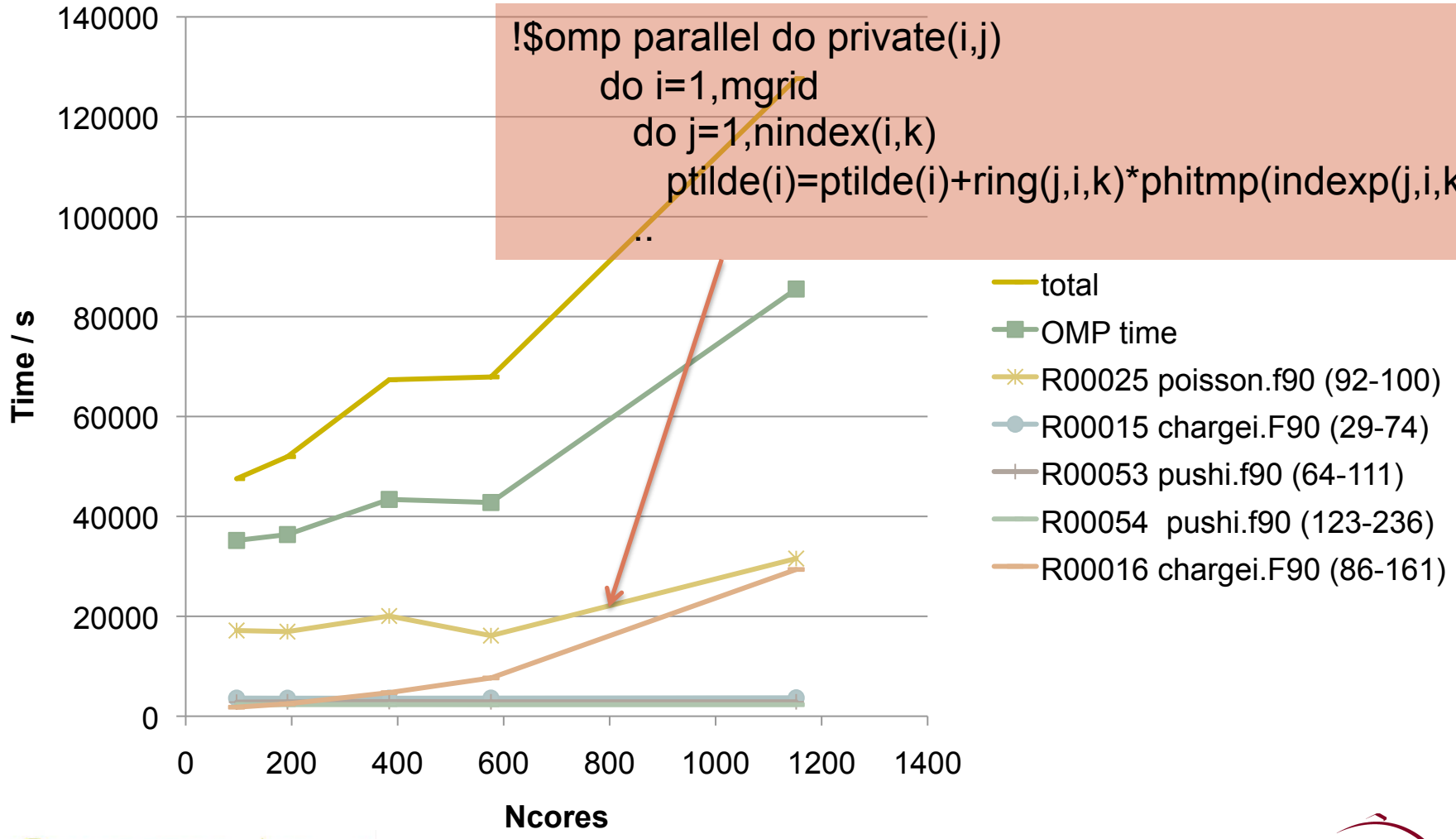
Strong Scaling cont.

```
!$omp parallel do private(i,j)
        do i=1,mi
              dnitmp(i,threadid) =
…
!$omp critical
   do k=1,nthreads
      do j=1,mgrid
              dni(j) = dni(j)+dnitmp(j,k)
.
```



Strong Scaling cont.

```
!$omp parallel do private(i,j)
        do i=1,mgrid
           do j=1,nindex(i,k)
              ptilde(i)=ptilde(i)+ring(j,i,k)*phitmp(indexp(j,i,k))
           ..
```



PARATEC - First Principles Electronic Structure Calculations

- First Principles: Full quantum mechanical treatment of electrons
- Gives accurate results for Structural and Electronic Properties of Materials, Molecules, Nanostructures
- Computationally very expensive (eg. grid of > 1 million points for each electron)
- Density Functional Theory (DFT) Plane Wave Based (Fourier) methods probably largest user of Supercomputer cycles in the world.
- ~13% total NERSC workload including single "biggest" code VASP
- PARAllel Total Energy Code (PARATEC) proxy in the NERSC6 benchmark suite

ab initio Density Functional Theory (Kohn 98 Nobel Prize)

Many Body Schrodinger Equation (exponential scaling)

$$\{-\sum_i \frac{1}{2}\nabla_i^2 + \sum_{i,j} \frac{1}{|r_i - r_j|} + \sum_{i,I} \frac{Z}{|r_i - R_I|}\}\Psi(r_1,..r_N) = E\Psi(r_1,..r_N)$$

Kohn Sham Equation (65): The many body ground state problem can be mapped onto a single particle problem with the same electron density and a different effective potential (cubic scaling).

$$\{-\frac{1}{2}\nabla^2 + \int \frac{\rho(r')}{|r - r'|}dr' + \sum_I \frac{Z}{|r - R_I|} + V_{XC}\}\psi_i(r) = E_i\psi_i(r)$$

$$\rho(r) = \sum_i |\psi_i(r)|^2 = |\Psi(r_1,..r_N)|^2$$

Use Local Density Approximation (LDA) for $V_{XC}[\rho(r)]$ (good Si,C)

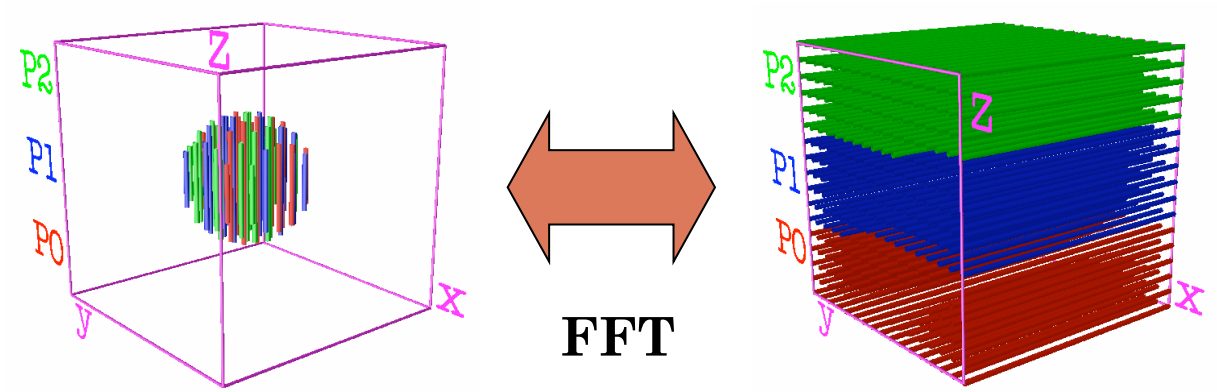
Load Balancing & Parallel Data Layout

- Wavefunctions stored as spheres of points (100-1000s spheres for 100s atoms)
- Data intensive parts (BLAS) proportional to number of Fourier components
- Pseudopotential calculation, Orthogonalization scales as N^3 (atom system)
- FFT part scales as $N^2 \log N$

Data distribution: load balancing constraints (Fourier Space):

- each processor should have same number of Fourier coefficients (N^3 calcs.)
- each processor should have complete columns of Fourier coefficients (3d FFT)

$$-\frac{1}{2}\nabla^2\psi_i(r)$$



$$V(r)$$

Give out sets of columns of data to each processor

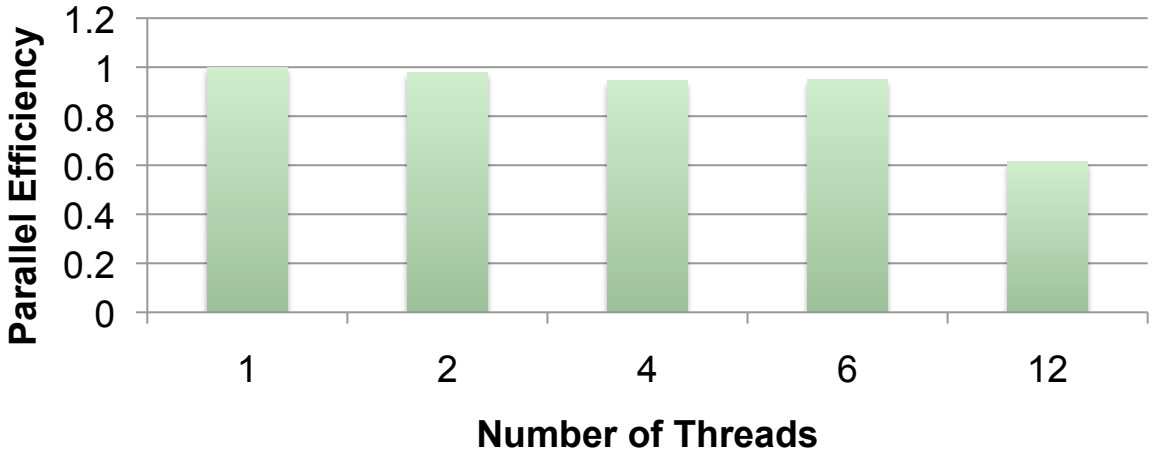
Basic algorithm & Profile of Paratec

- Orthogonalization – ZGEMM
  - N^3
- FFT
  - N ln N

- At small concurrencies ZGEMM dominates at large FFT

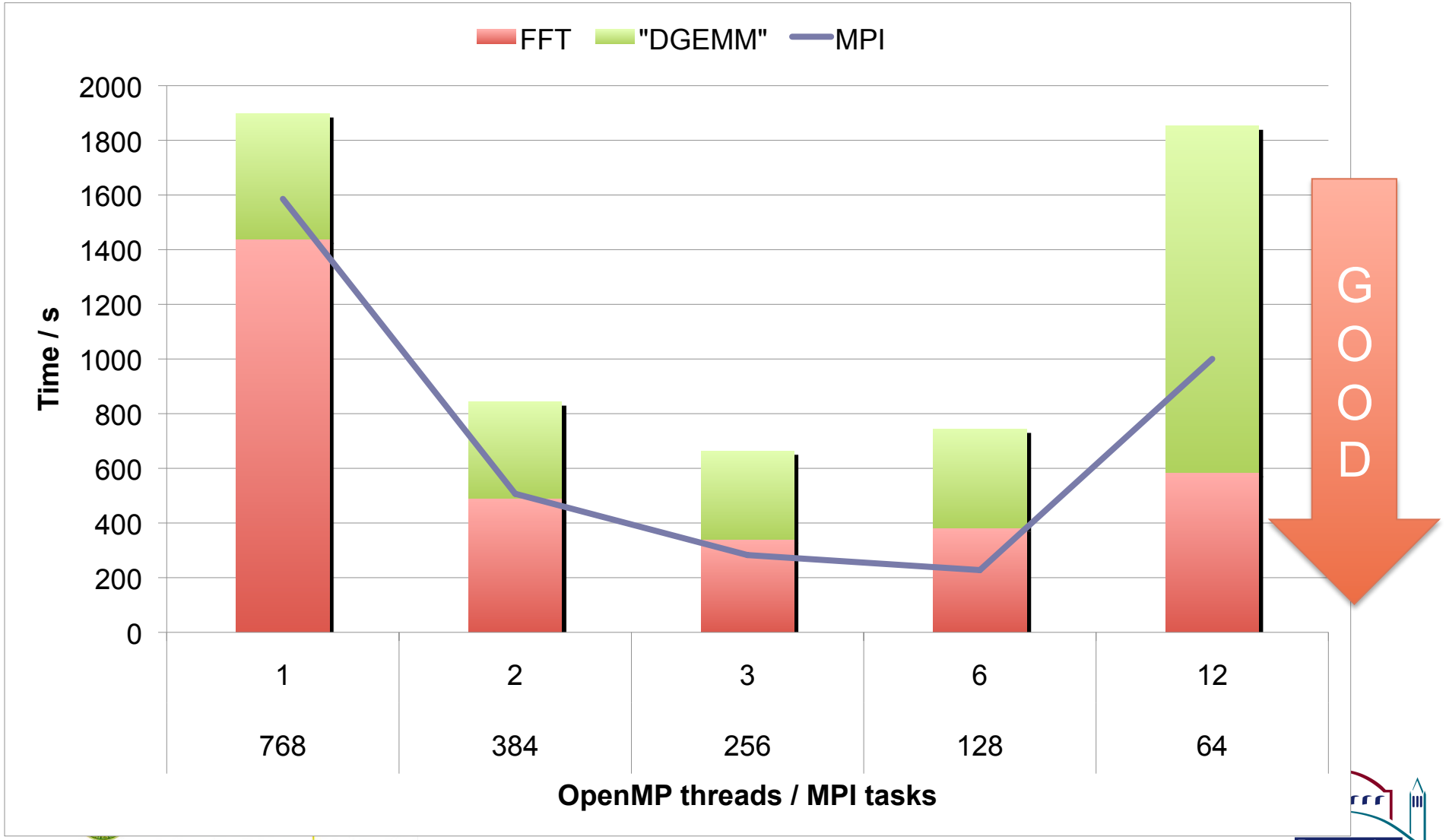
What OpenMP can do for Paratec?

- ZGEMM very amenable to threading

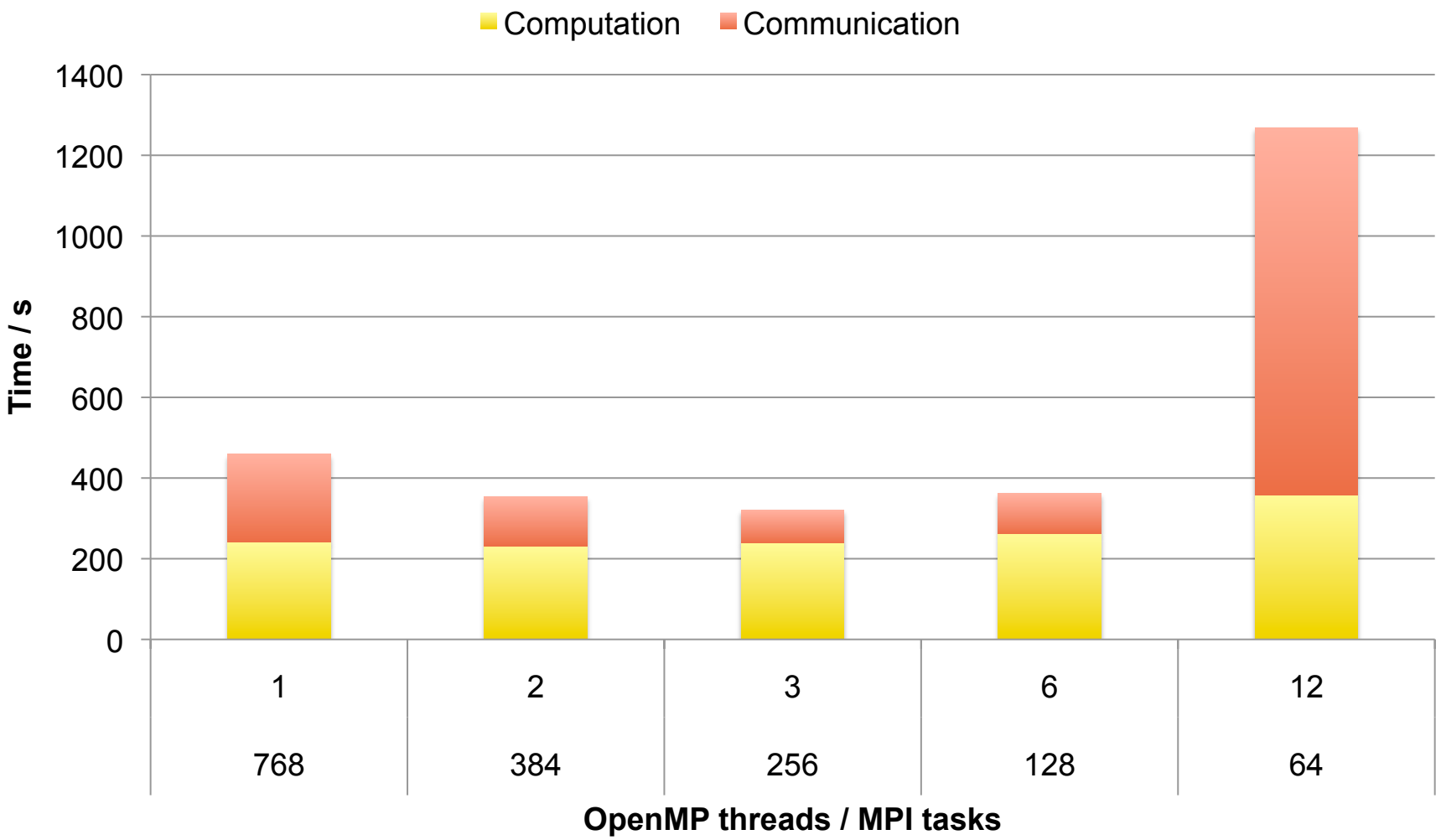


- FFT also
  - Can thread FFT library calls themselves
  - Can 'package' individual FFT's so that messages are combined -> more efficient communication

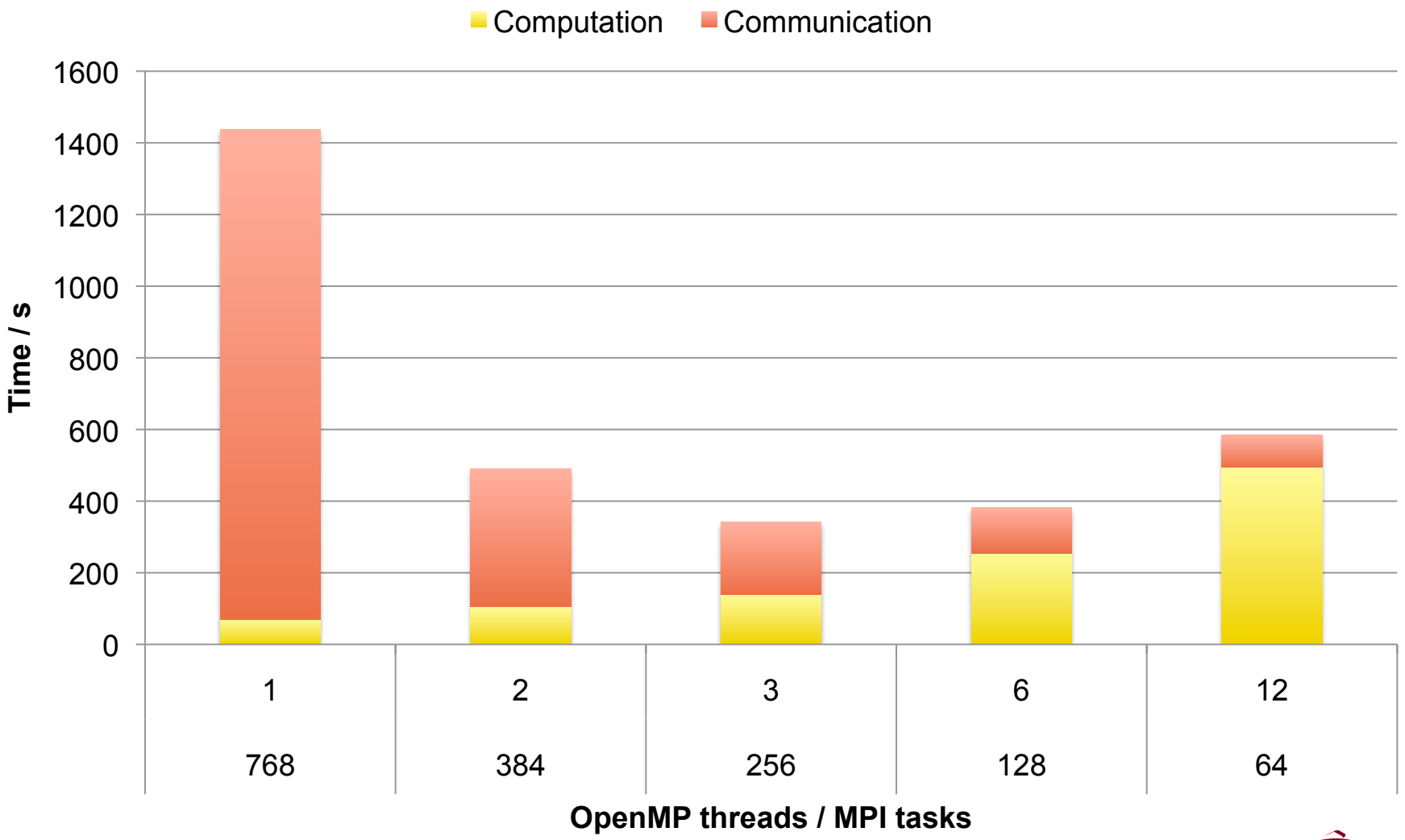
Paratec MPI+OpenMP Performance



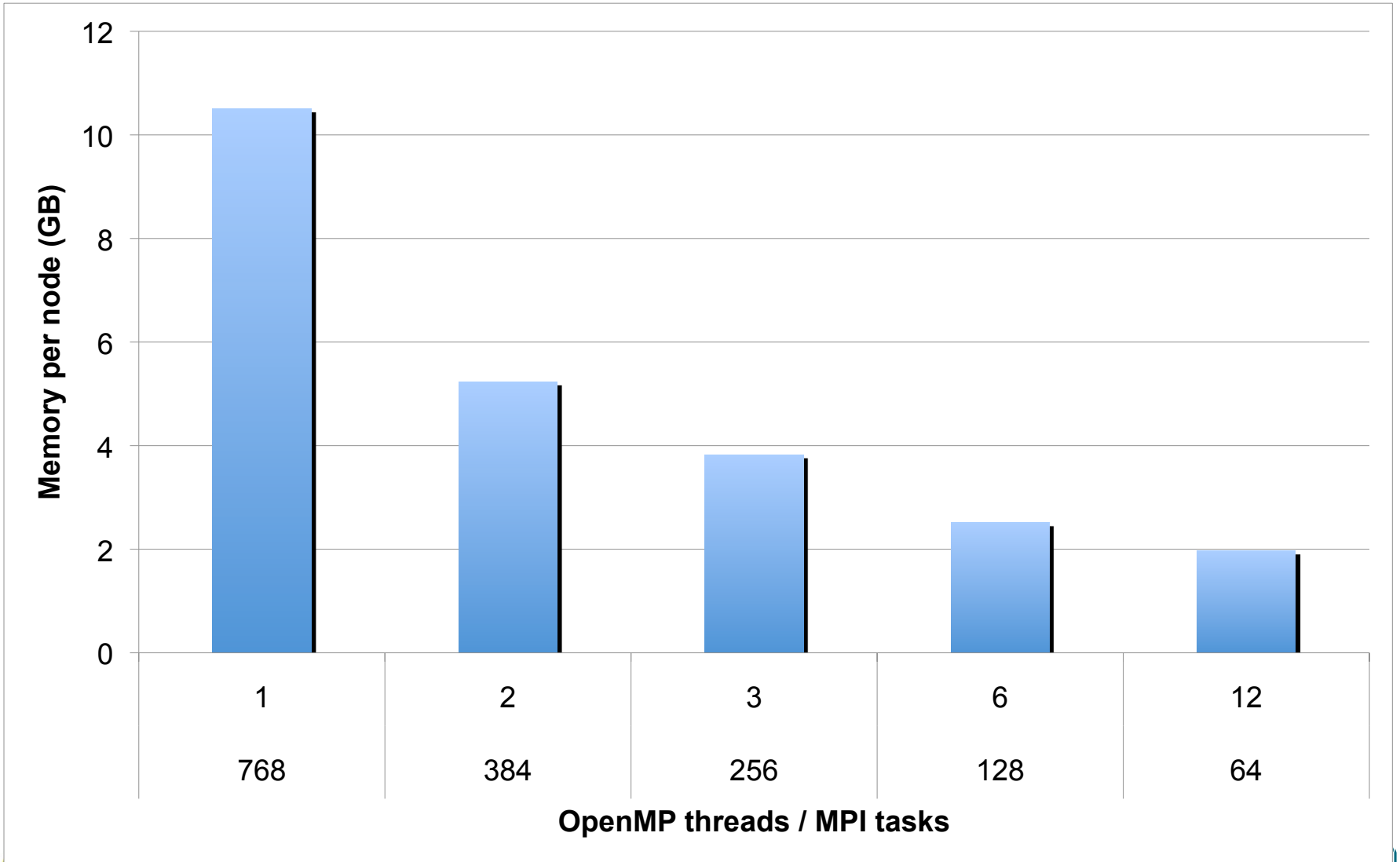
Parallel "ZGEMM"



FFT Breakdown



PARATEC - Memory Usage

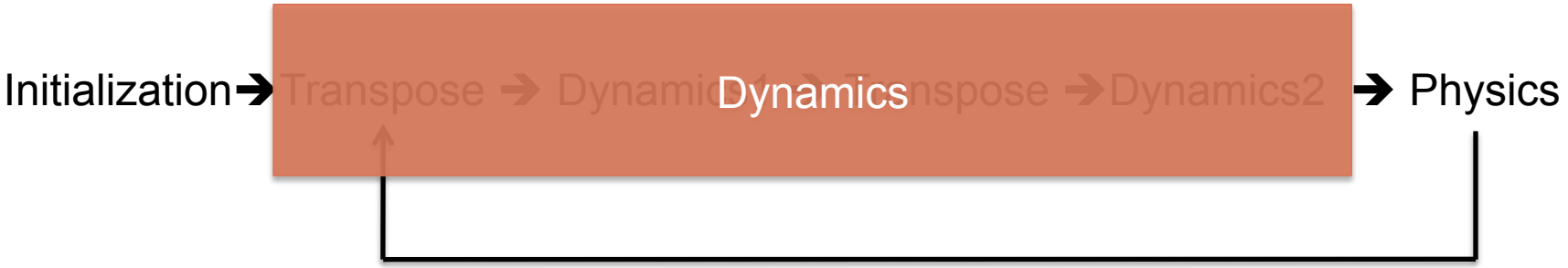


Finite Volume Community Atmospheric Model- fvCAM

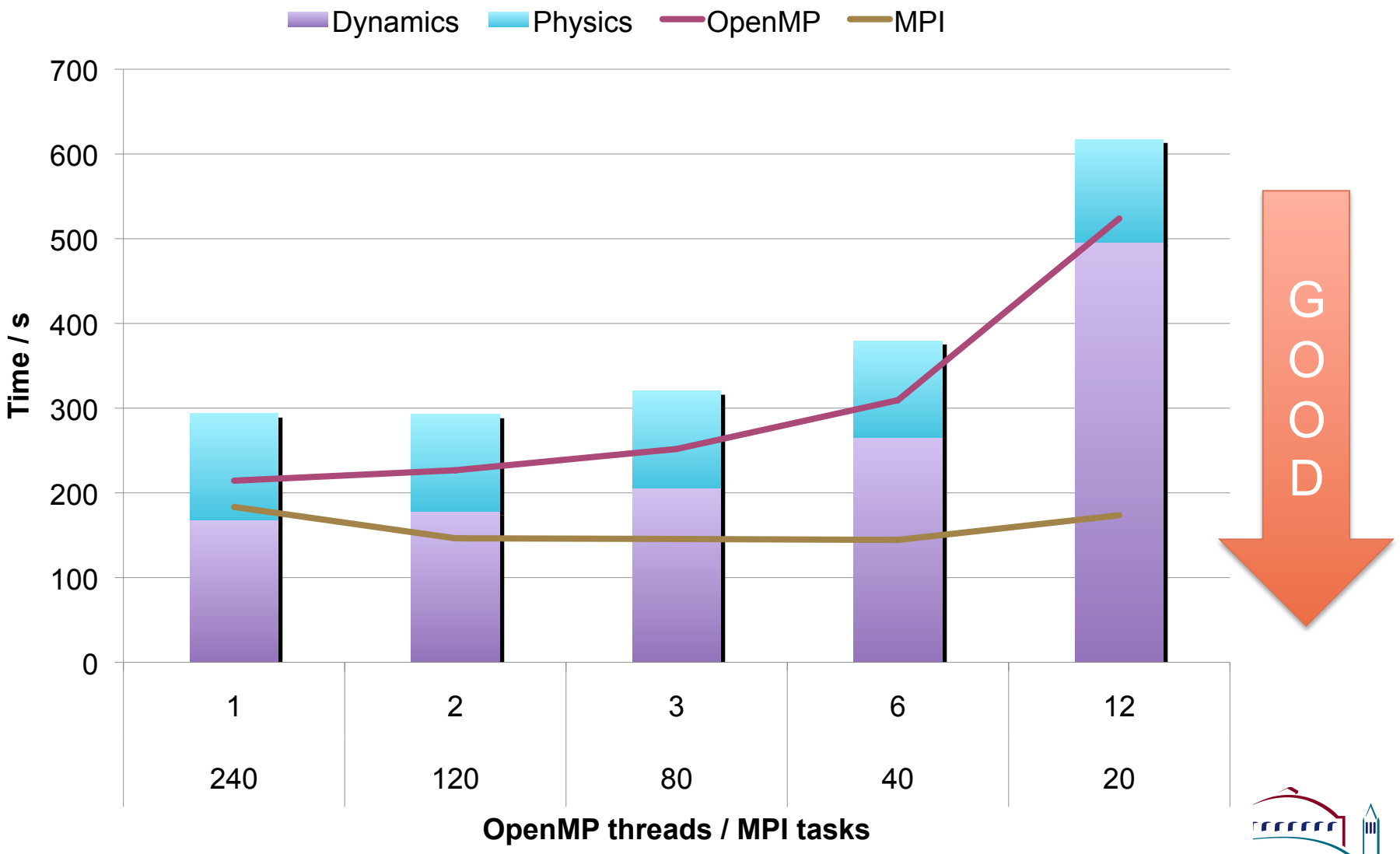
- Dynamics and physics use separate decompositions
  - physics utilizes a 2D longitude/latitude decomposition
  - dynamics utilizes multiple decompositions
    - FV dynamics 2D block latitude/vertical and 2D block longitude/latitude
- Decompositions are joined with transposes
- Each subdomain is assigned to at most one MPI task
- Additional parallelism via OpenMP ~500 OpenMP directives over 72 .F90 files

fvCAM coordinate system

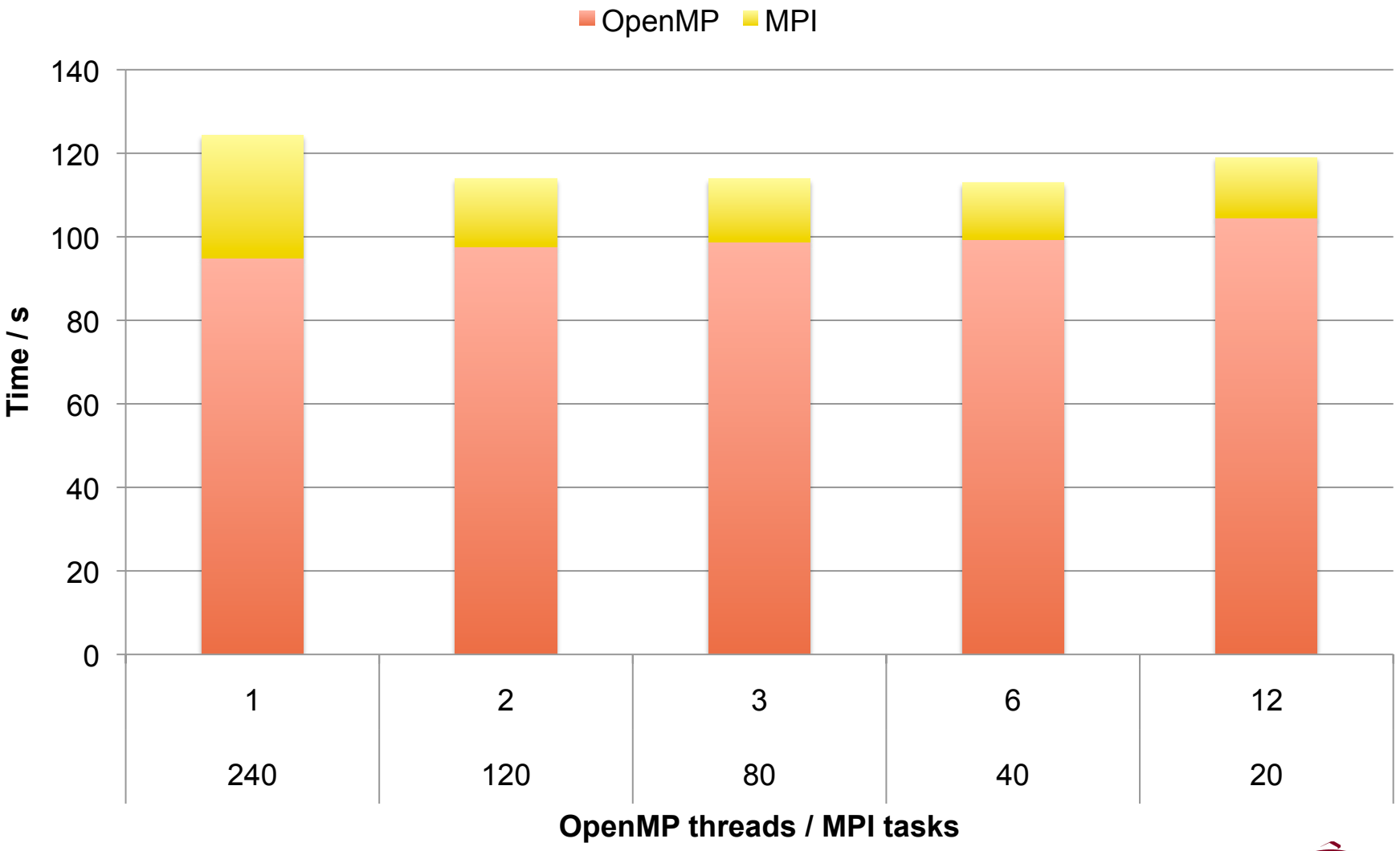
- 576x361x28 grid (Longitude x Latitude x Vertical) (X Y Z)
- Original problem definition - 240 MPI tasks - 60(Y) x 4(Z,X) decomposition
- Dynamics uses Lat-Vert and Lat-Long
- Physics uses Lat-Long decomposition



fvCAM MPI+OpenMP Performance



fvCAM Physics

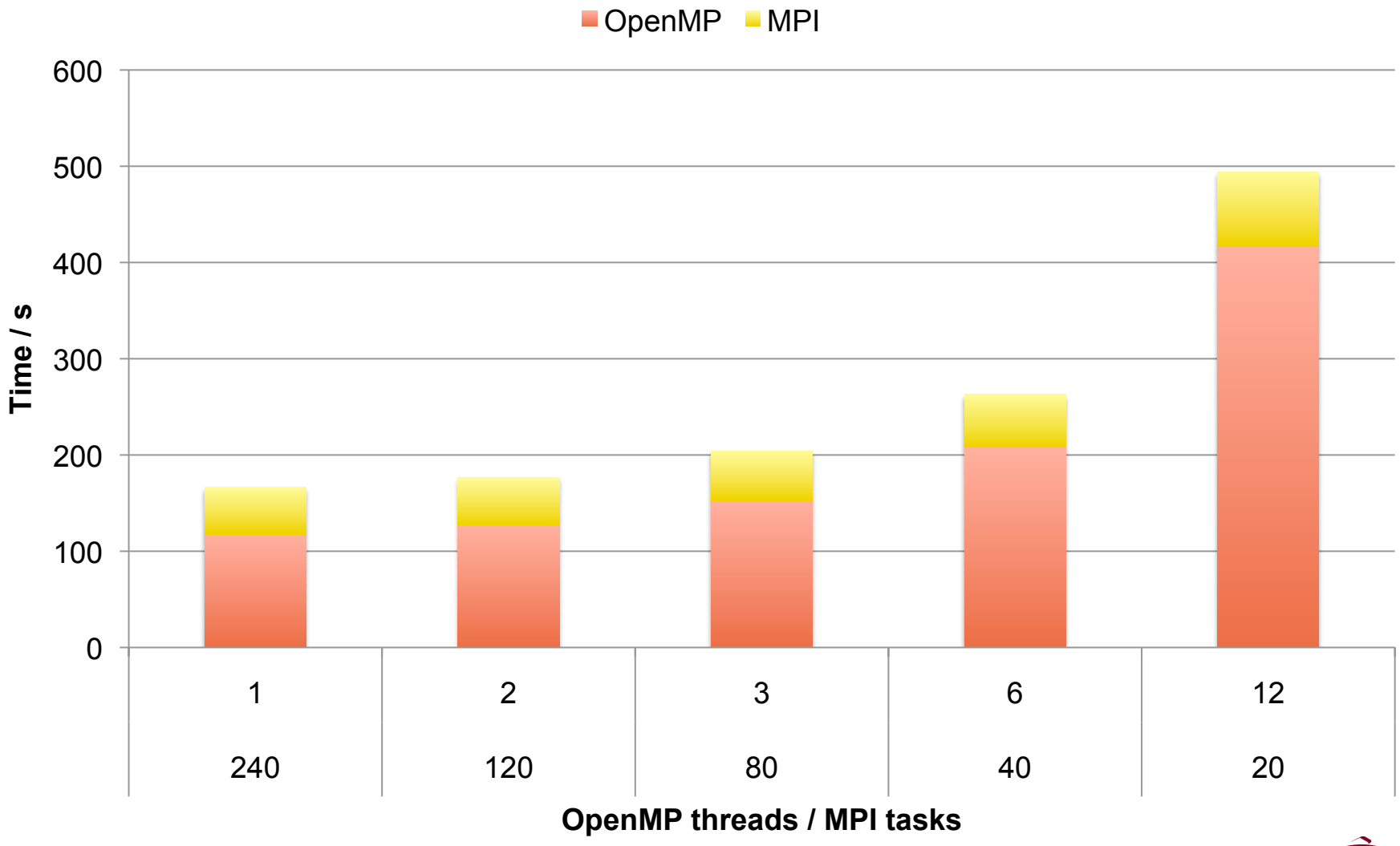


CAM: Physics

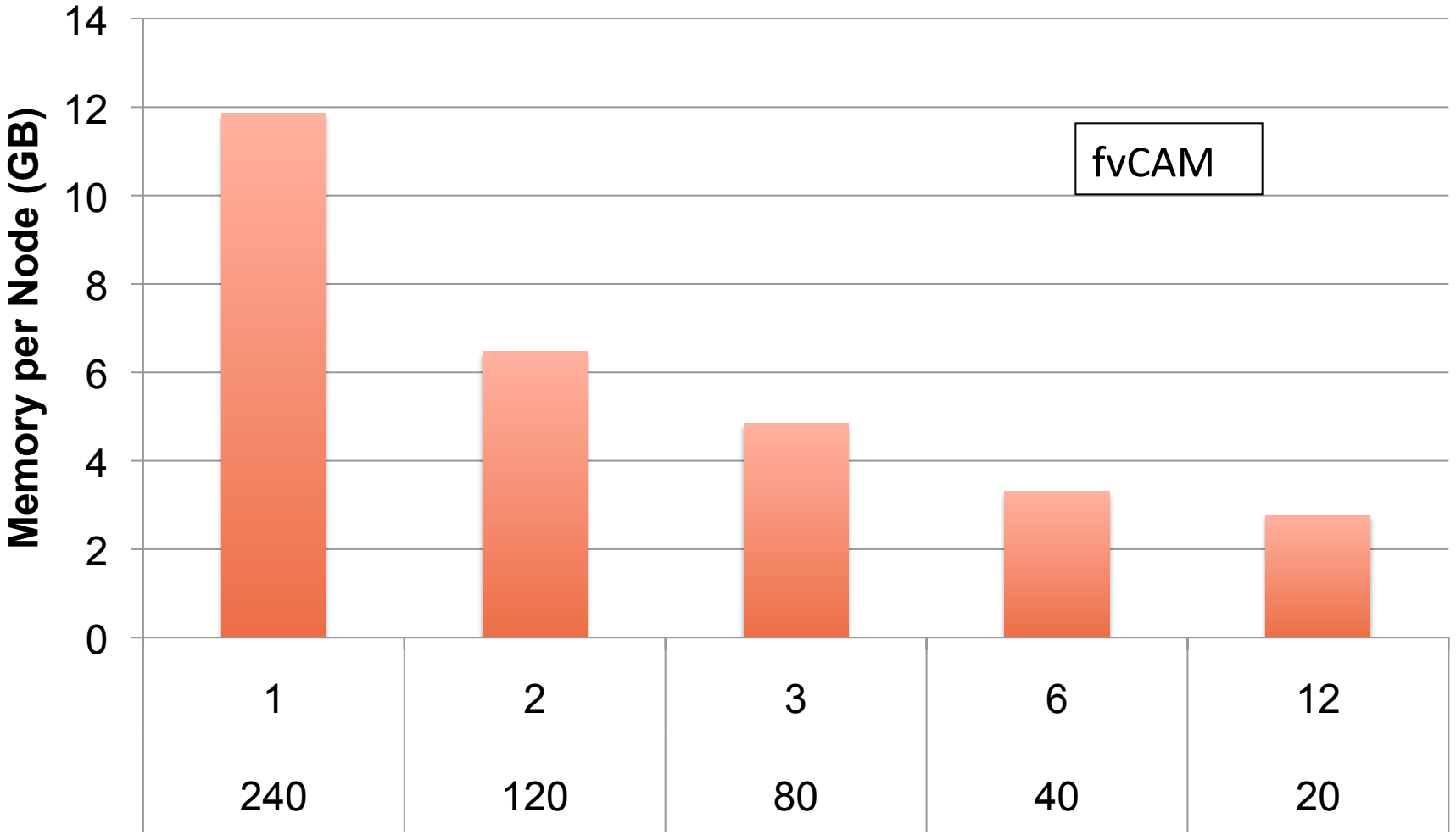
- Columnar processes (typically parameterized) such as precipitation, cloud physics, radiation, turbulent mixing lead to large amounts of work per thread and high efficiency

```
!$OMP PARALLEL DO PRIVATE (C)
do c=begchunk, endchunk
     call tphysbc (ztodt, pblht(1,c), tpert(1,c),
    snowhland(1,c),phys_state(c),phys_tend(c), pbuf,fsds(1,c)....
 enddo
```

fvCAM - Dynamics



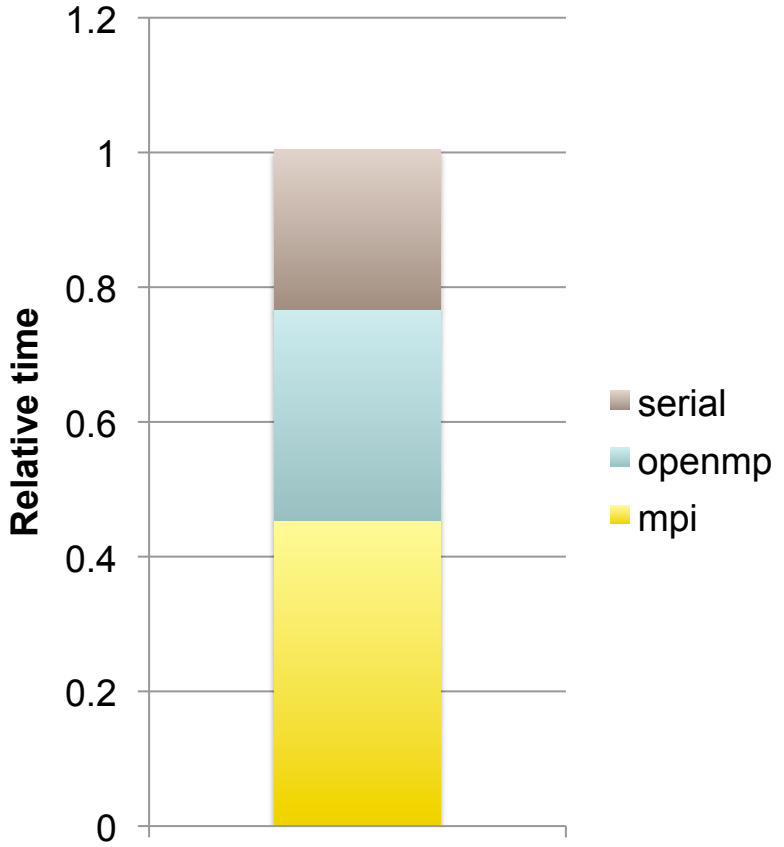
Less Memory Usage with OpenMP Compared to Flat MPI



Advanced OpenMP techniques

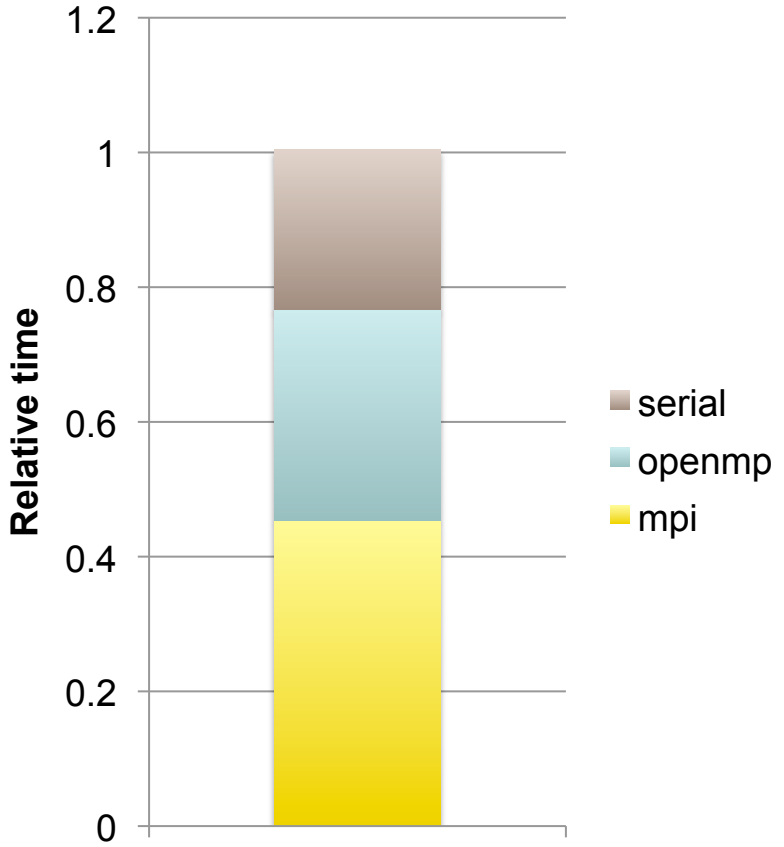
GTC - Shifte Routine

- Which e^- to move?
- Pack e^- to be moved
- Communicate # e^- to move
- Repack non-moving e^-
- Send/Recv e^-
- And again….



Shifte Routine

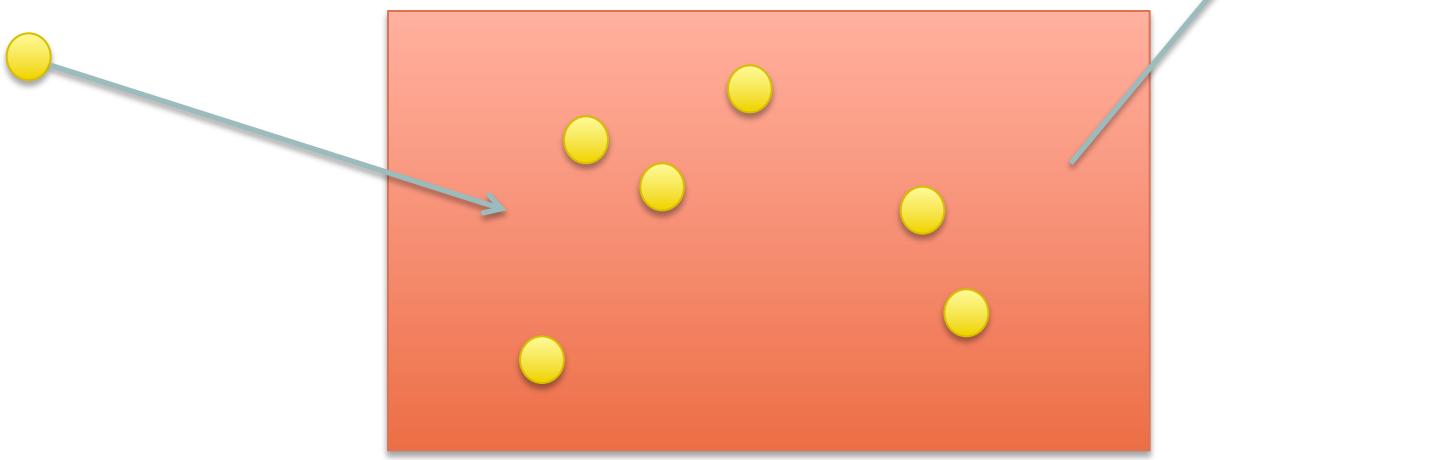
- Which e- to move? ✔
- Pack e- to be moved ✗
- Communicate # e- to move ✗
- Repack non-moving e- ✗
- Send/Recv e- ✗
- And again…..



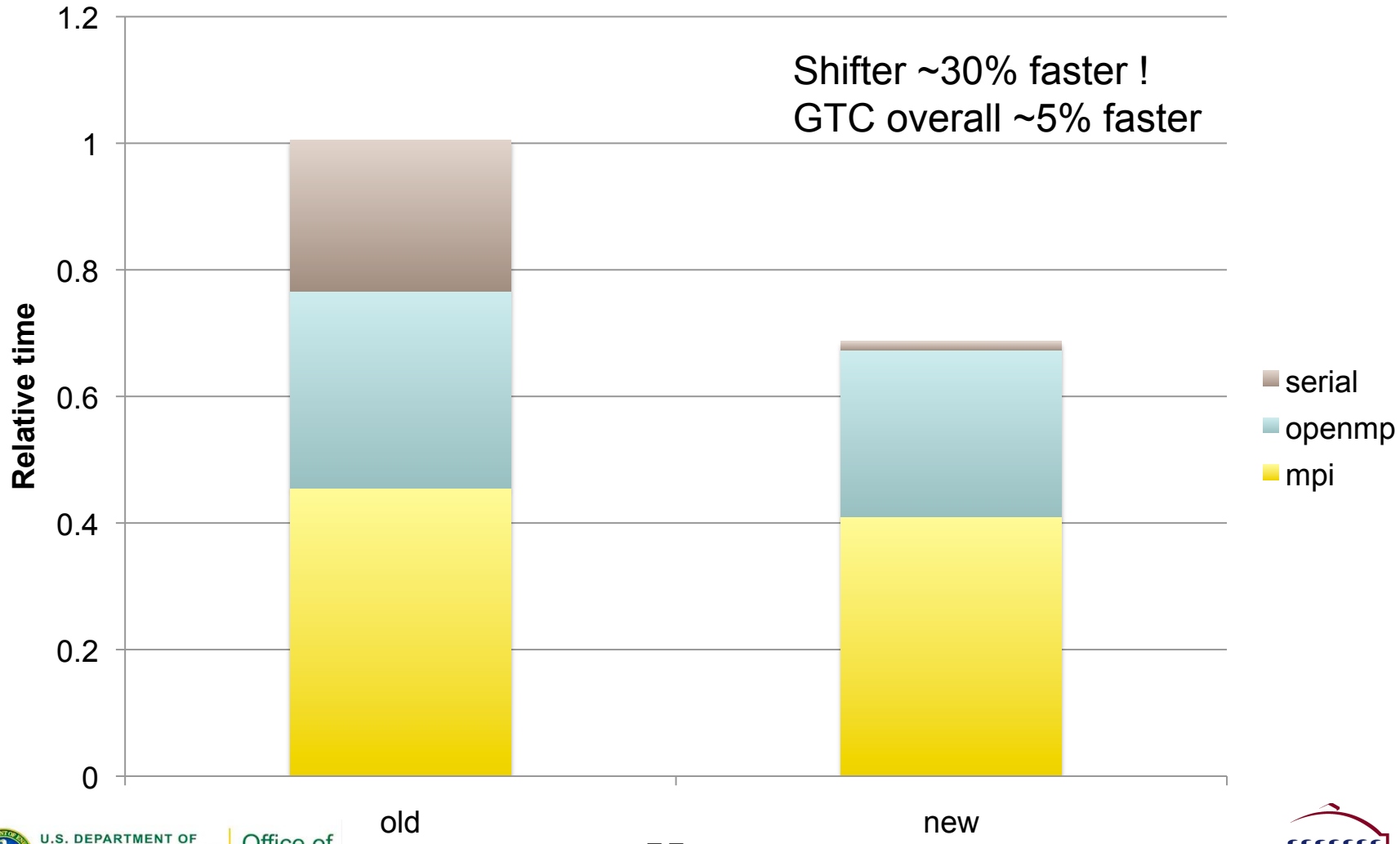
OPENMP tasking

Idle Threads Can
Execute Tasks in pool

Executing Thread Encountering Task
Region Adds Task to pool
#pragma omp task



Tasking - Results



Summary

- OpenMP + MPI can be faster than pure MPI – and is often comparable in performance
- Beware NUMA !
  - Don't use >6 OpenMP threads unless absolutely necessary or you can 'first-touch' perfectly
- Beware !$OMP critical !
  - Unless you absolutely have to
- Need Holistic view of your codes performance bottlenecks
  - Adding more cores may not help –transpose

Advice to NERSC Users - Hopper

1. Should I use OpenMP?
   - + Need to save memory and have duplicated structures across MPI tasks
   - + Routine that parallelises with OPENMP only – Poisson routine in GTC
   - – Reduction operations – charge & push in GTC
   - – Threads can be hard – locks, race conditions
2. How hard is it to change my code?
   - Easier than serial to MPI
   - Easier than UPC/ CAF ?
3. How do I know if it's working or not?
   - – IPM, OMPP, TAU, HPCToolkit, Craypat

Lessons for NERSC Users- Longer Term

- Are you going to tell me in 3 years that I should have used CAF/UPC/Chapel ?
- Uncertainty about Future Machine model
  - GPU programming model – streaming
  - Many lightweight cores
- OpenMP as it stands today is not ideally suited to either model
  - Mend it? Broken ?? (GPU flavor of OMP)

Next Steps for COE

- **Phase 1 completing**
  - **Application studies completed**
  - **Final technical report by end of year**

- **Phase 2 starting up**
  - **Apply lessons from phase1 to leading application codes**
    - *VASP: largest user base at NERSC (create OpenMP implementation)*
  - **Selecting advanced programming models for study**
  - **Selecting representative applications and kernels from NERSC-6 applications**
    - *GTS: represents broad class of PIC algorithms (create CAF version)*