Calculating π in Parallel Using MPI

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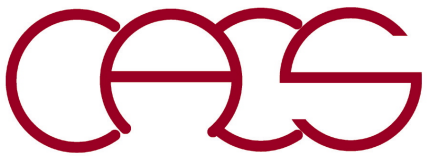
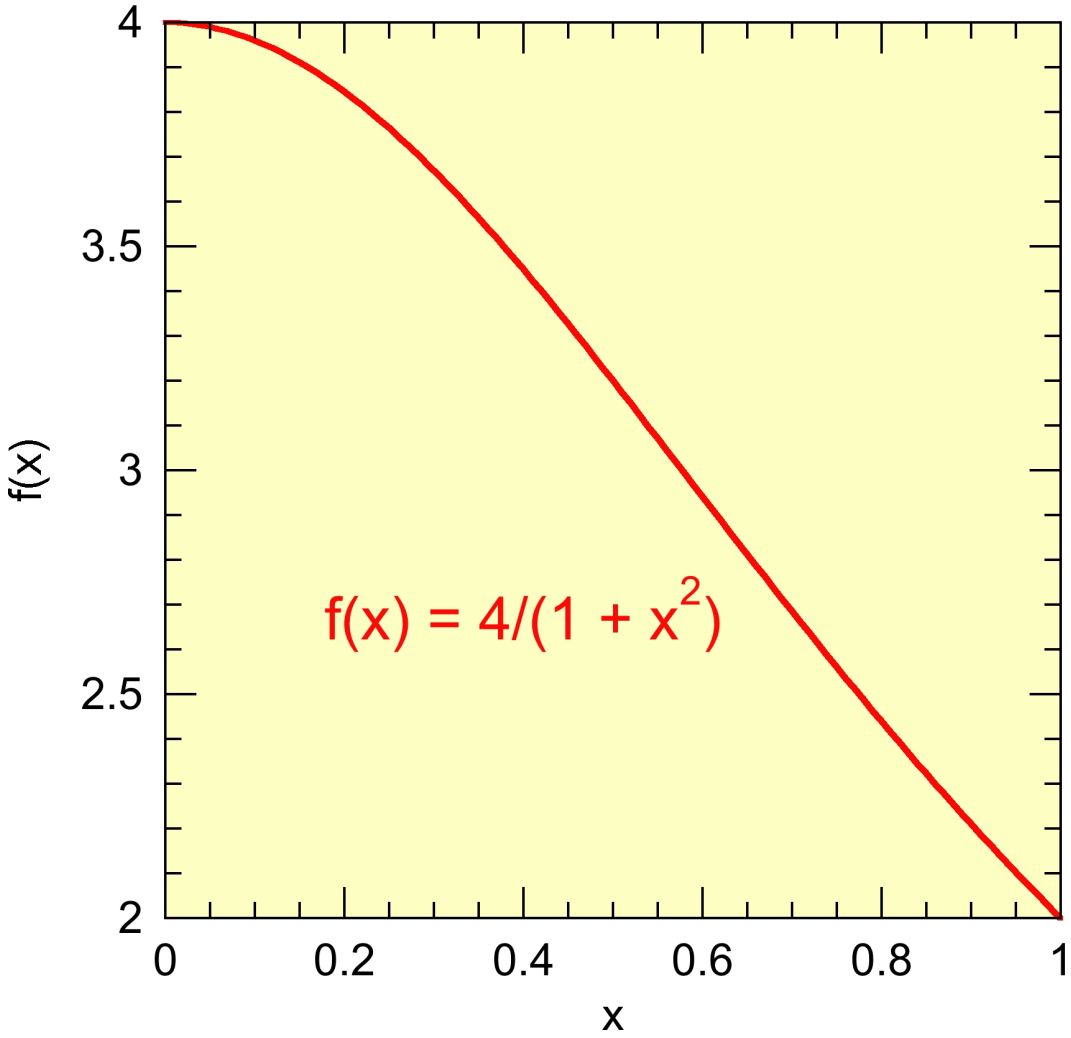
Objectives

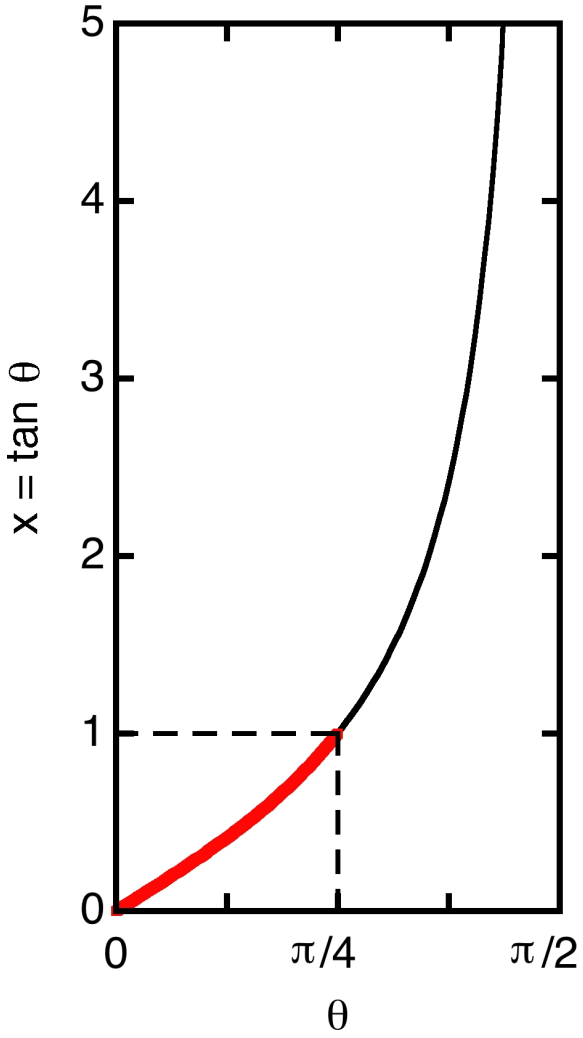
1. **Task decomposition (parallel programming = who does what)**
2. **Scalability analysis**



Integral Representation of π

$$\int_0^1 dx \frac{4}{1+x^2} = \int_0^{\pi/4} \frac{d\theta}{\cos^2\theta} \frac{4}{1+\tan^2\theta} = \int_0^{\pi/4} 4d\theta = \pi$$





Numerical Integration of π

- **Integration**

$$\int_0^1 dx \frac{4}{1+x^2} = \pi$$

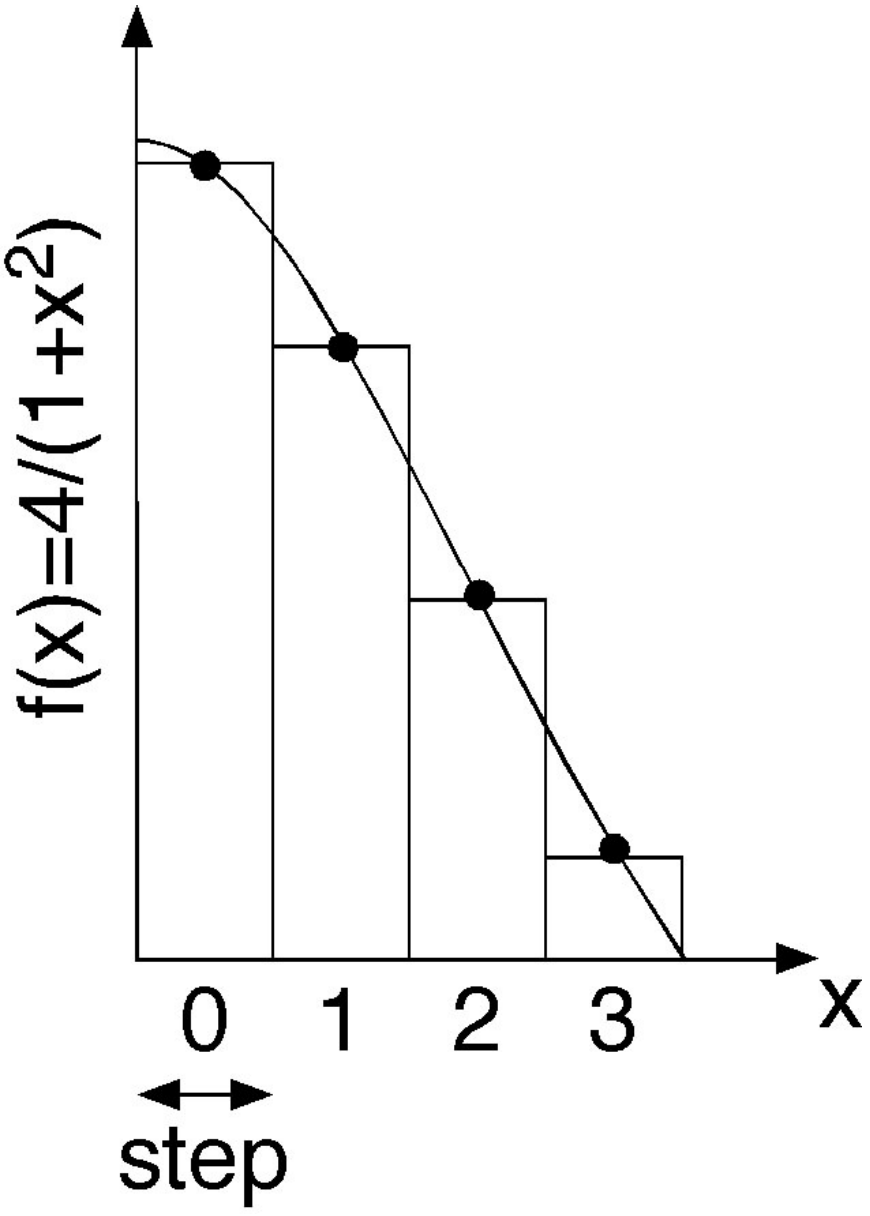
- **Discretization:**

$\Delta = 1/N$: `step = 1/NBIN`

$x_i = (i+0.5)\Delta$ $(i = 0,\ldots,N\text{-}1)$

$$\sum_{i=0}^{N-1} \frac{4}{1+x_i^2}\Delta \cong \pi$$

```
#include <stdio.h>
#define NBIN 10000000
void main() {
  int i; double step,x,sum=0.0,pi;
  step = 1.0/NBIN;
  for (i=0; i<NBIN; i++) {
    x = (i+0.5)*step;
    sum += 4.0/(1.0+x*x);
  }
  pi = sum*step;
  printf( "PI = %f\n" ,pi);
}
```

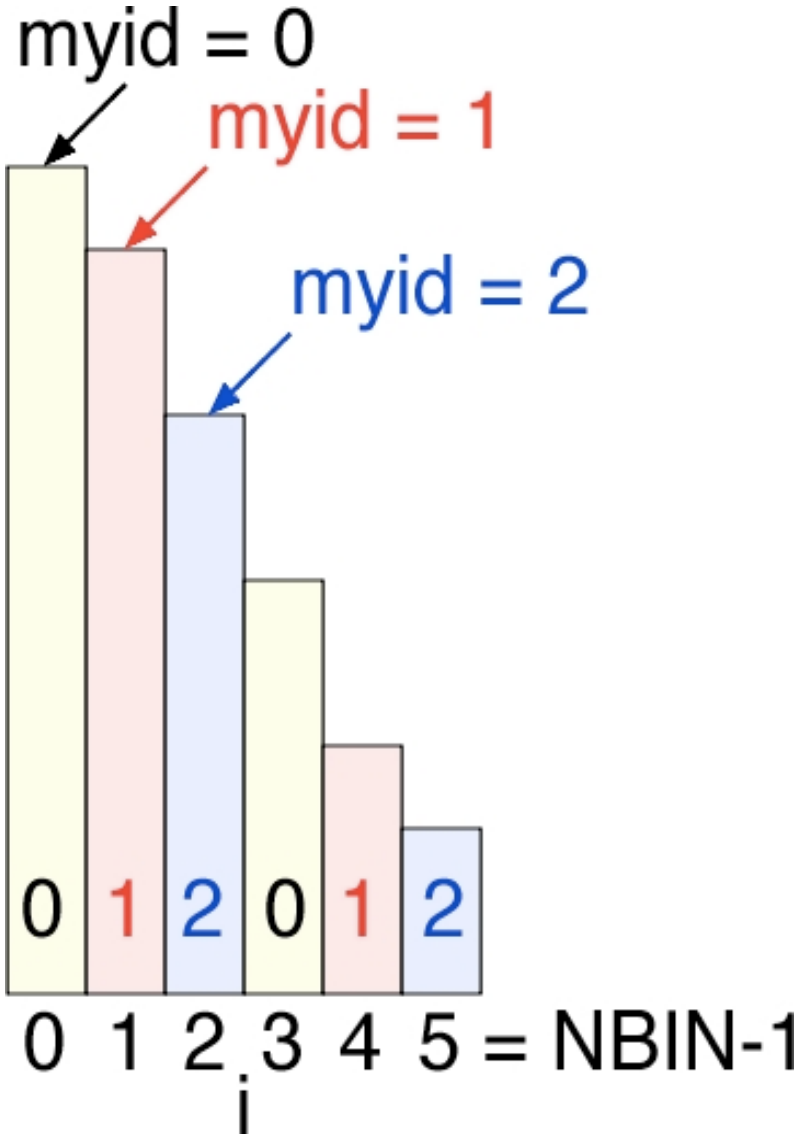


Parallelization: Who Does What?

Interleaved assignment of quadrature points (bins) to MPI processes

Single program multiple data (SPMD)

```
...
for (i=myid; i<NBIN; i+=nprocs)
{
  x = (i+0.5)*step;
  sum += 4.0/(1.0+x*x);
}
partial = sum*step;
pi = global_sum(partial);
...
```




```
MPI_Comm_rank(MPI_COMM_WORLD,&myid)
```

myid = MPI rank

nprocs = Number of MPI processes

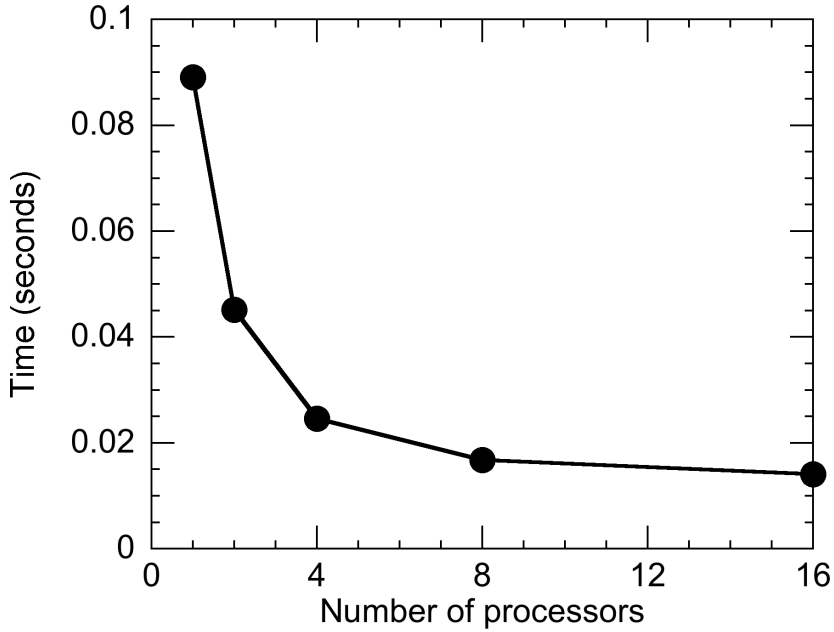
```
MPI_Comm_size(MPI_COMM_WORLD,&nprocs)
```

- Use `double MPI_Wtime()` to measure the running time in seconds

Parallel Running Time

global_pi.c: NBIN = 10^7, on HPC

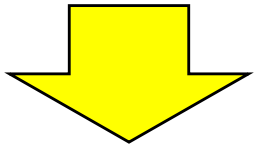
```
#SBATCH --ntasks-per-node=16
#SBATCH --nodes=1
...
srun -n $SLURM_NTASKS --mpi=pmi2 ./global_pi
srun -n               8 --mpi=pmi2 ./global_pi
srun -n               4 --mpi=pmi2 ./global_pi
srun -n               2 --mpi=pmi2 ./global_pi
srun -n               1 --mpi=pmi2 ./global_pi
```



How Efficient Is the Parallel Program?

Scalability Analysis

- **Parallel computing = Solving a big problem (*W*) in a short time (*T*) using many processors (*P*)**



- **How *W*, *T* & *P* scale with each other?**
- **How to define the efficiency of a parallel program?**

Parallel Efficiency

- **Execution time: $T(W,P)$**
  W: Workload
  P: Number of processors

- **Speed:** $$S(W,P) = \frac{W}{T(W,P)}$$

- **Speedup:** $$S_P = \frac{S(W_P,P)}{S(W_1,1)} = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)}$$

- **Efficiency:** $$E_P = \frac{S_P}{P} = \frac{W_P T(W_1,1)}{P W_1 T(W_P,P)}$$

How to scale W_P with P?

Fixed Problem-Size Scaling

$W_P = W$—constant (strong scaling)

- **Speedup:** $S_P = \dfrac{T(W,1)}{T(W,P)}$

$$S_P = \frac{S(W_P,P)}{S(W_1,1)} = \frac{W_P T(W_1,1)}{W_1 T(W_P,P)}$$

- **Efficiency:** $E_P = \dfrac{T(W,1)}{PT(W,P)}$

$$E_P = \frac{S_P}{P} = \frac{W_P T(W_1,1)}{PW_1 T(W_P,P)}$$

- **Amdahl's law:** f **(= sequential fraction of the workload) limits the asymptotic speedup**

$$T(W,P) = fT(W,1) + \frac{(1-f)T(W,1)}{P}$$

$$\therefore S_P = \frac{T(W,1)}{T(W,P)} = \frac{1}{f + (1-f)/P}$$

$$\therefore S_P \to \frac{1}{f} \quad (P \to \infty)$$

Isogranular Scaling

$W_P = Pw$ (weak scaling)
w = constant workload per processor (granularity)

- **Speedup:** $S_P = \dfrac{S(P \bullet w, P)}{S(w,1)} = \dfrac{P \bullet w / T(P \bullet w, P)}{w / T(w,1)} = \dfrac{P \bullet T(w,1)}{T(P \bullet w, P)}$

- **Efficiency:** $E_P = \dfrac{S_P}{P} = \dfrac{T(w,1)}{T(P \bullet w, P)}$

$$S_P = \frac{S(W_P, P)}{S(W_1, 1)} = \frac{W_P T(W_1, 1)}{W_1 T(W_P, P)}$$

$$E_P = \frac{S_P}{P} = \frac{W_P T(W_1, 1)}{P W_1 T(W_P, P)}$$

Analysis of Global_Pi Program

- **Workload ∝ Number of quadrature points, N (or `NBIN` in the program)**
- **Parallel execution time on P processors:**
  - **> Local computation ∝ N/P**

```
for (i=myid; i<N; i+=P){
  x = (i+0.5)*step; partial += 4.0/(1.0+x*x);
}
```

  - **> Butterfly computation/communication in global() ∝ log$P$**

```
for (l=0; l<log2P; ++l) {
  partner = myid XOR 2^l;
  send mydone to partner;
  receive hisdone from partner;
  mydone += hisdone
}
```

$$T(N,P) = T_{\text{comp}}(N,P) + T_{\text{global}}(P)$$
$$= \alpha \frac{N}{P} + \beta \log P$$

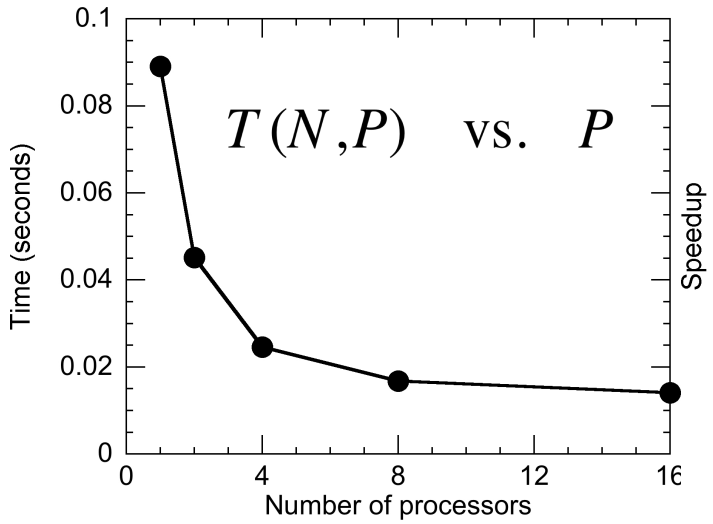
Fixed Problem-Size (Strong) Scaling

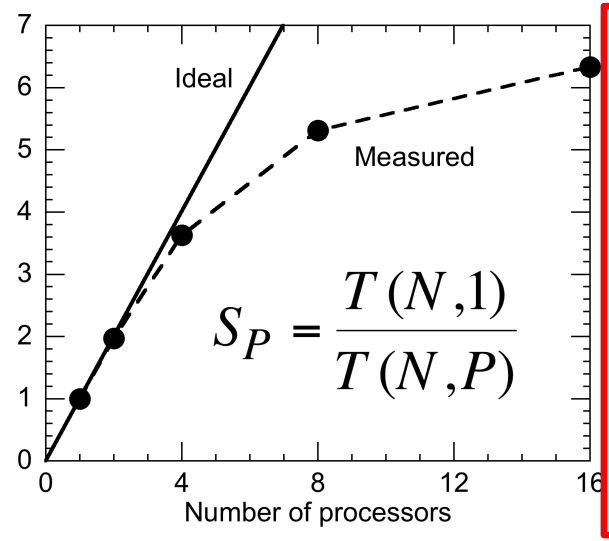
- **Speedup:**

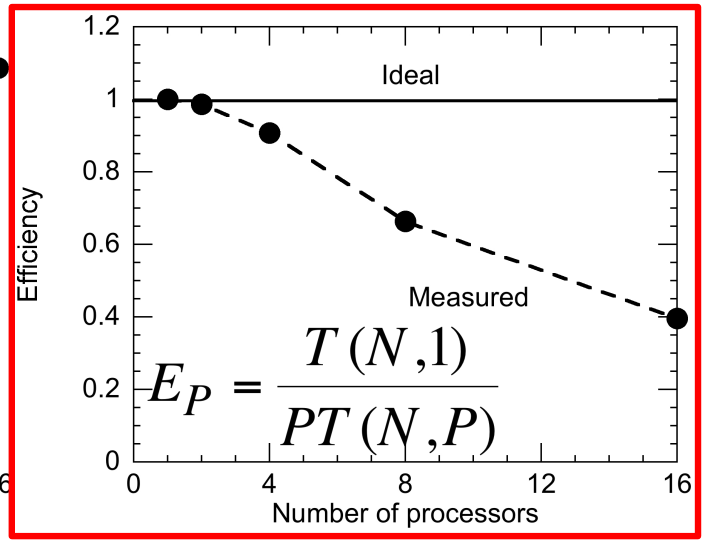
$$S_P = \frac{T(N,1)}{T(N,P)} = \frac{\alpha N}{\alpha \frac{N}{P} + \beta \log P} = \frac{P}{1 + \frac{\beta}{\alpha}\frac{P \log P}{N}}$$

- **Efficiency:**

$$E_P = \frac{S_P}{P} = \frac{1}{1 + \frac{\beta}{\alpha}\frac{P \log P}{N}}$$



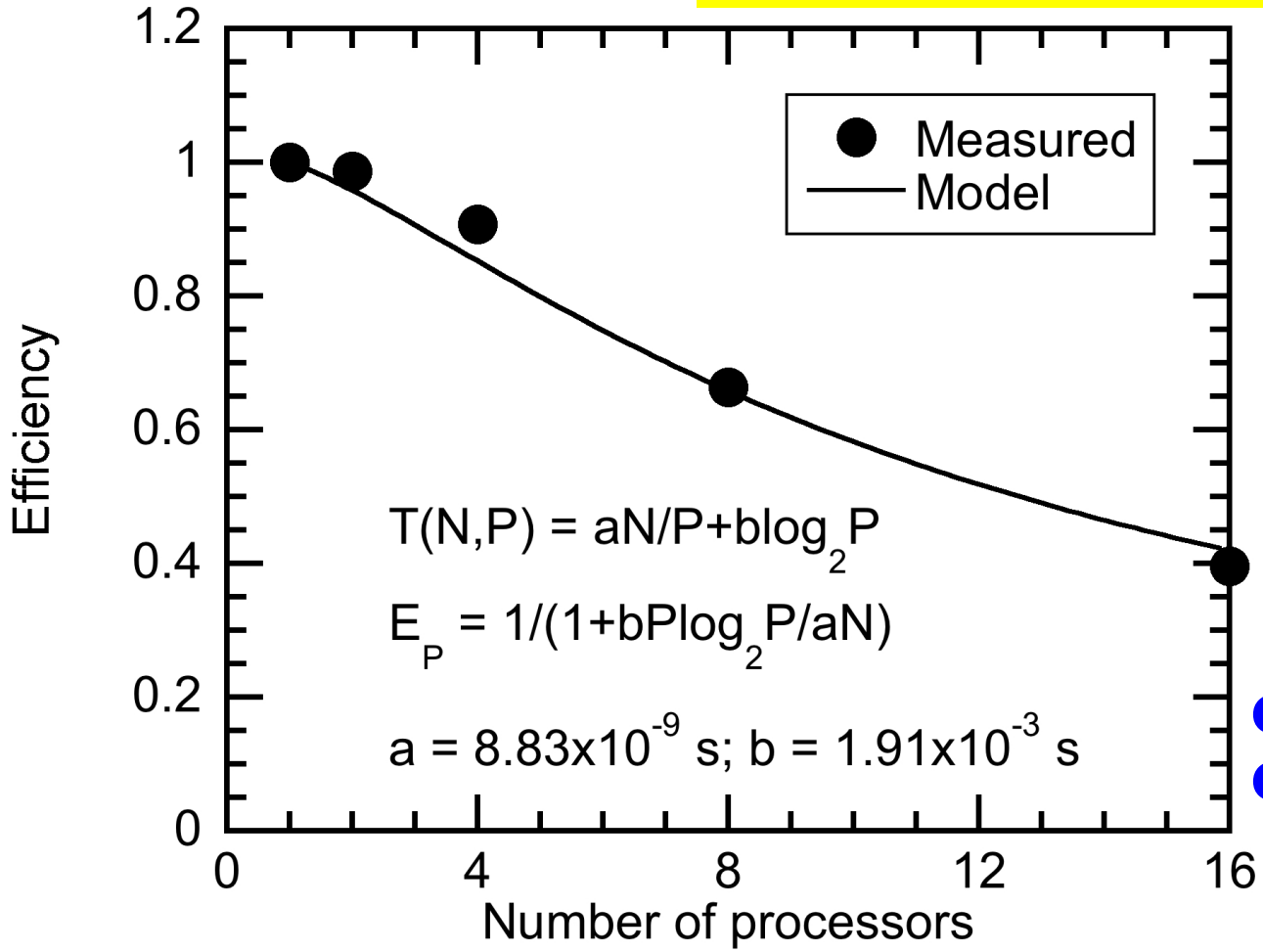




global_pi.c: $N = 10^7$, on HPC

Fixed Problem-Size Scaling

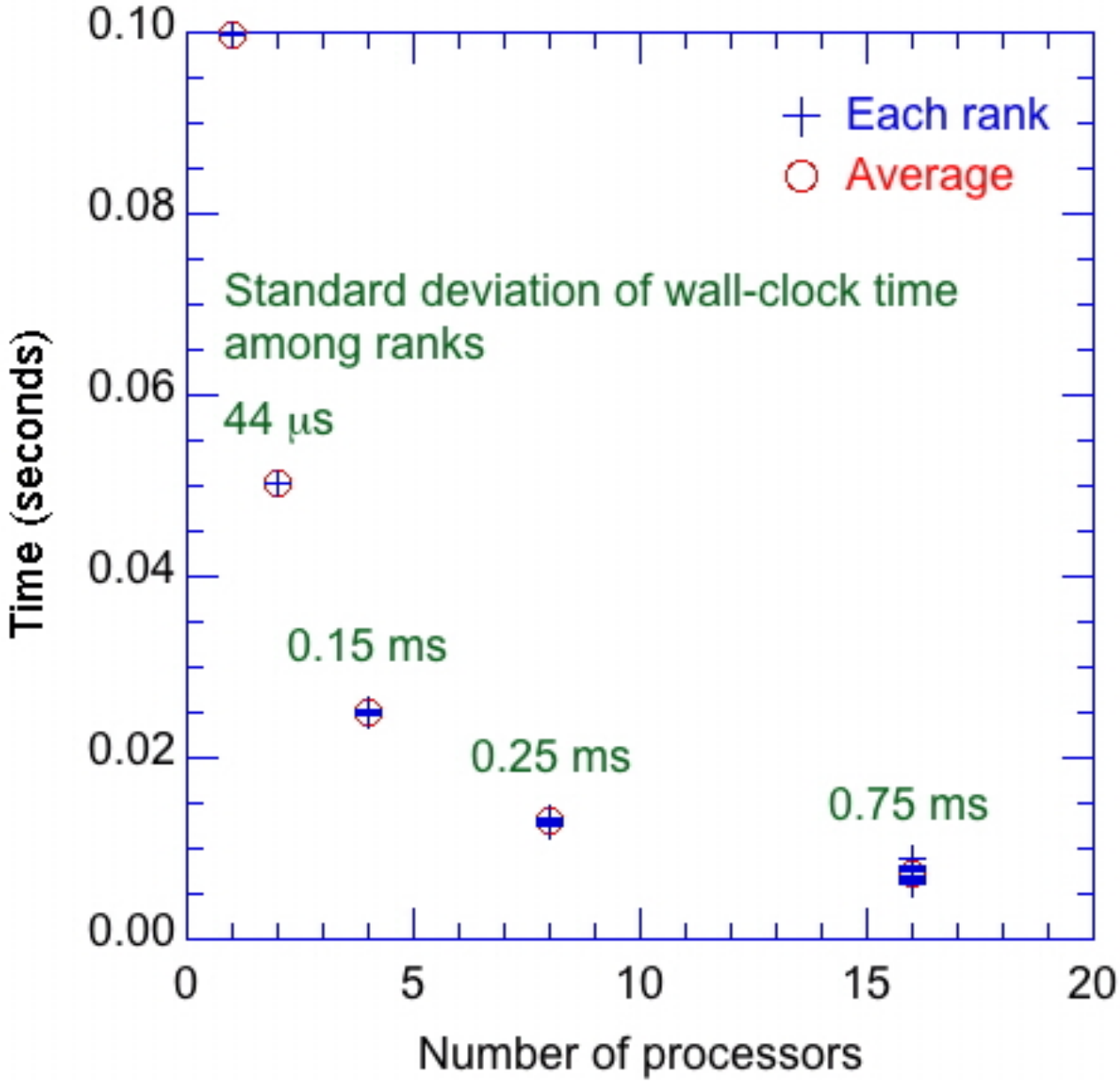
- **Speedup model:** $E_P = \frac{S_P}{P} = \frac{1}{1 + \frac{\beta}{\alpha}\frac{P\log P}{N}}$



Computation ~ ns
Communication ~ ms

global_pi.c: $N = 10^7$, on HPC

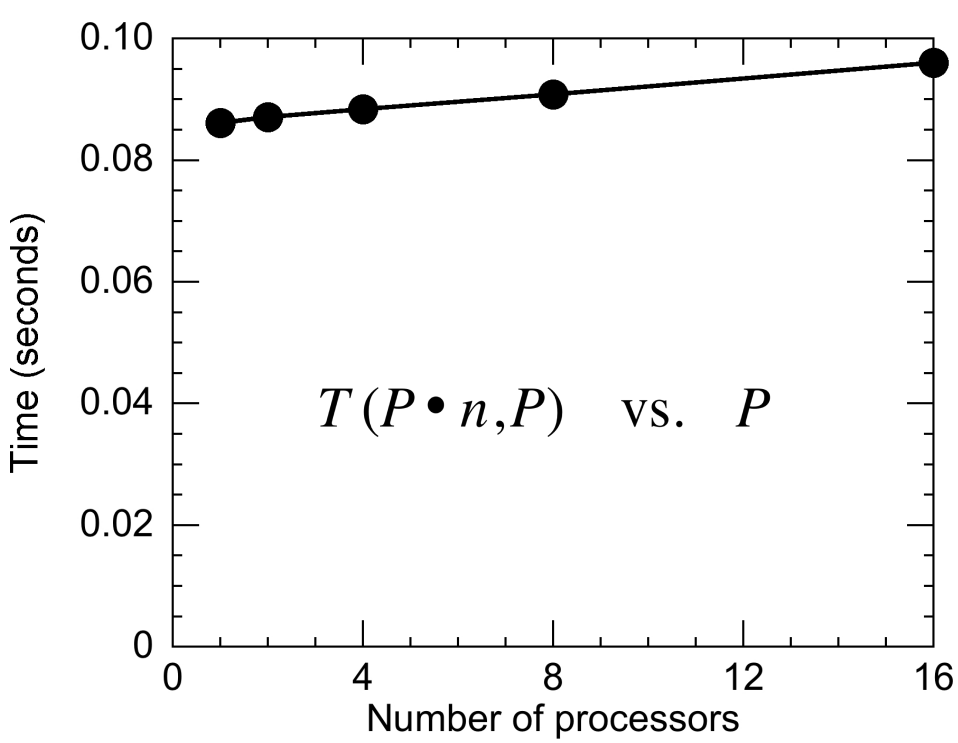
Runtime Variance among Ranks

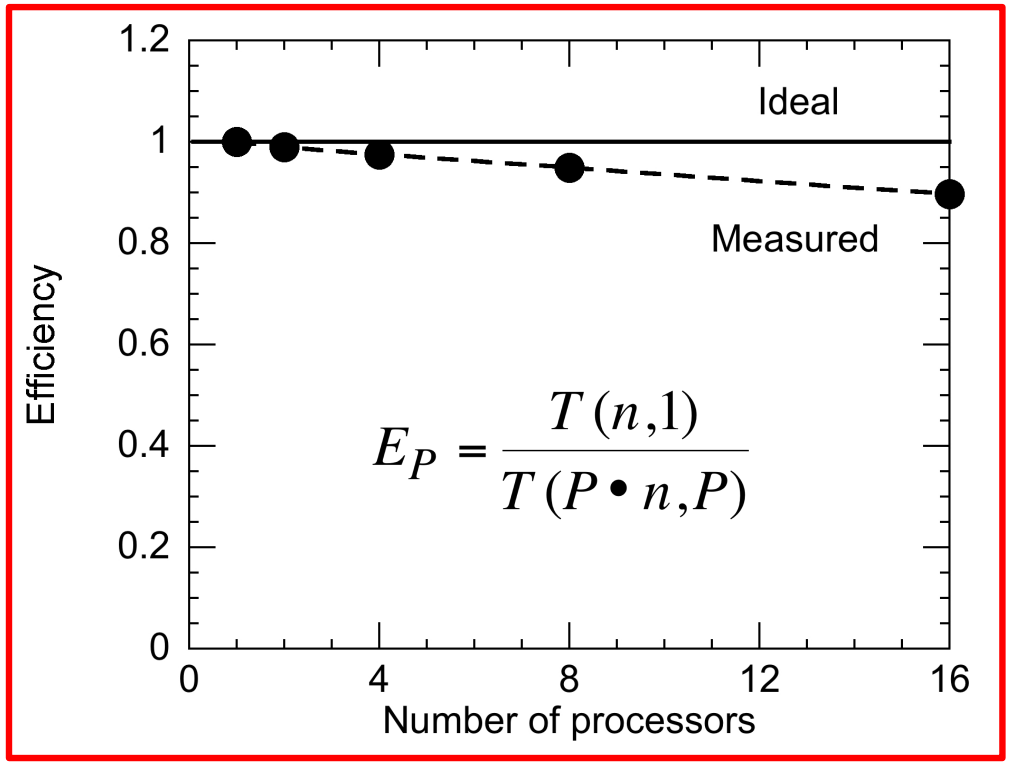


Isogranular (Weak) Scaling

- $n = N/P$ = constant
- **Efficiency:**

$$E_P = \frac{T(n,1)}{T(nP,P)} = \frac{\alpha n}{\alpha n + \beta \log P} = \frac{1}{1 + \frac{\beta}{\alpha n}\log P}$$

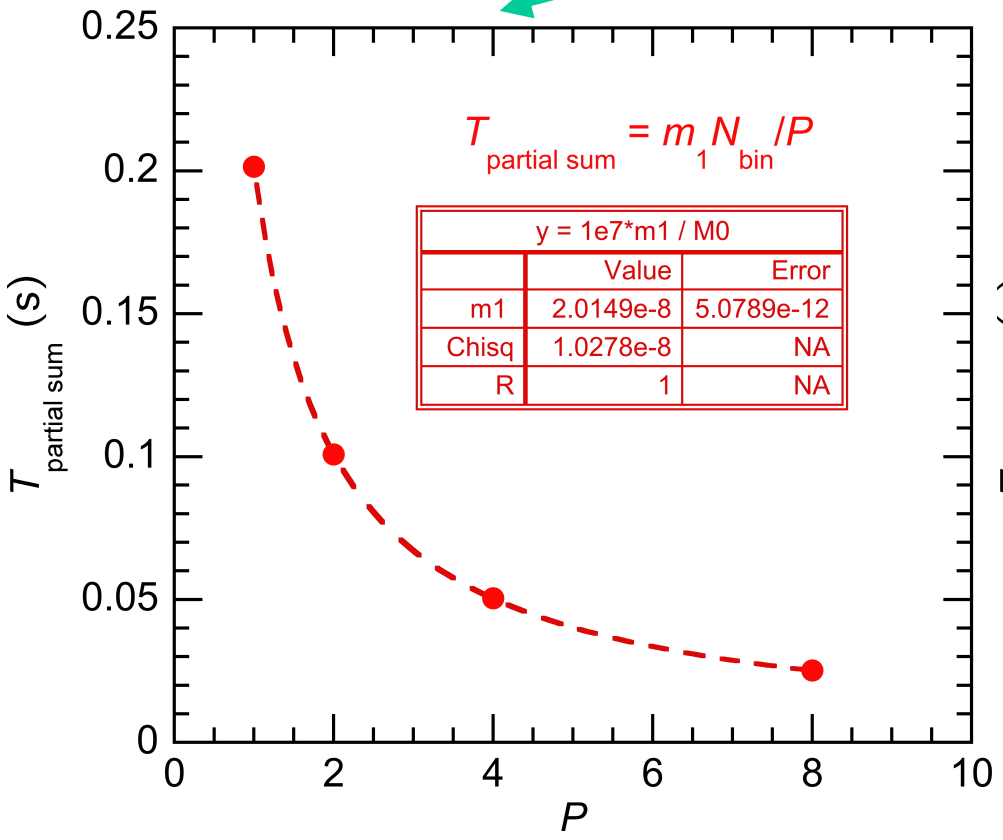




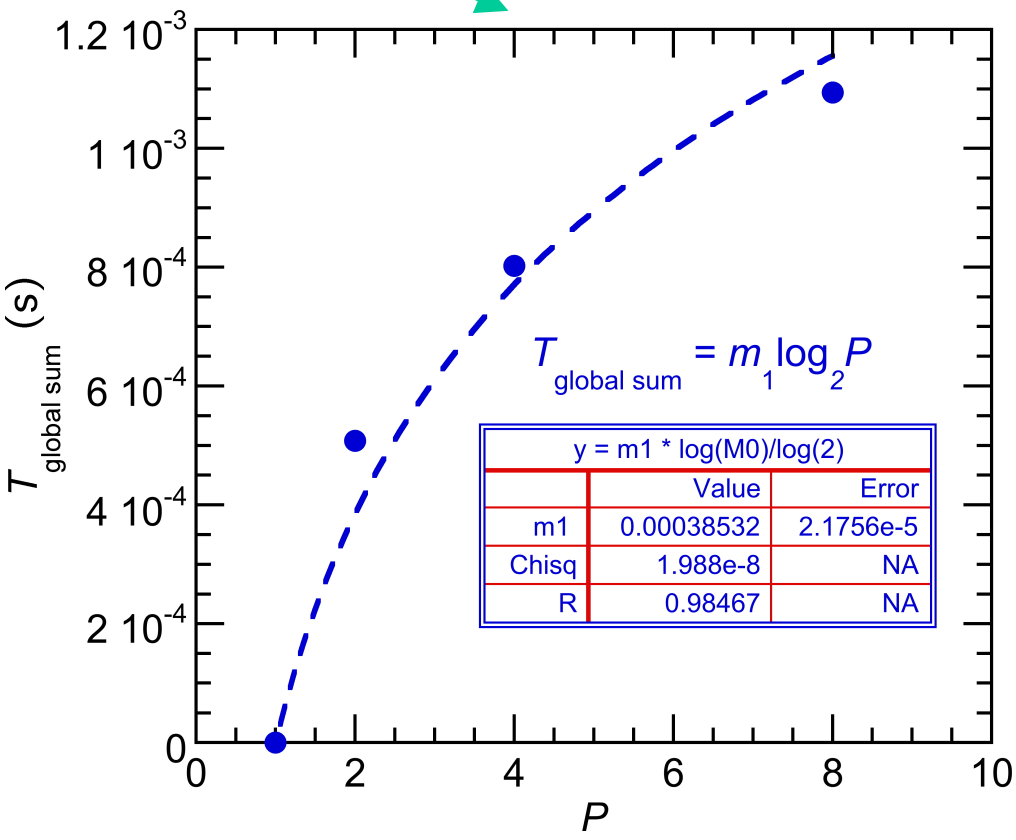
global_pi_iso.c: $N/P = 10^7$, on HPC

Fitting Fixed Problem-Size Scaling

$$T(N,P) = \alpha \frac{N}{P} + \beta \log_2 P$$



Computation ~ ns



Communication ~ ms

global_pi_breakdown.c: $N = 10^7$, on 3.0 GHz Xeon

Scalability Analysis: Example

Computer Physics Communications 219 (2017) 246–254

A derivation and scalable implementation of the synchronous parallel kinetic Monte Carlo method for simulating long-time dynamics

Hye Suk Byun [a], Mohamed Y. El-Naggar [a,b,c], Rajiv K. Kalia [a,d,e,f], Aiichiro Nakano [a,b,d,e,f,*], Priya Vashishta [a,d,e,f]

$$T(N,P) = T_{\text{comp}}(N,P) + T_{\text{comm}}(N,P) + T_{\text{global}}(P) = aN/P + b(N/P)^{2/3} + c\log P. \quad (6)$$

For isogranular scaling, the number of atoms per processor, $N/P = n$, is constant, and the isogranular parallel efficiency is

$$E_P = \frac{T(n,1)}{T(nP,P)} = \frac{an}{an + bn^{2/3} + c\log P} = \frac{1}{1 + \frac{b}{a}n^{-1/3} + \frac{c}{an}\log P}. \quad (7)$$

For fixed problem-size scaling, the global number of hemes, N, is fixed, and the speedup is given by

$$S_P = \frac{T(N,1)}{T(N,P)} = \frac{aN}{aN/P + b(N/P)^{2/3} + c\log P} = \frac{P}{1 + \frac{b}{a}\left(\frac{P}{N}\right)^{1/3} + \frac{c}{a}\frac{P\log P}{N}}, \quad (8)$$

and the parallel efficiency is

$$E_P = \frac{S_P}{P} = \frac{1}{1 + \frac{b}{a}\left(\frac{P}{N}\right)^{1/3} + \frac{c}{a}\frac{P\log P}{N}}. \quad (9)$$