Parameter Tuning of a Hybrid Treecode-FMM on GPUs

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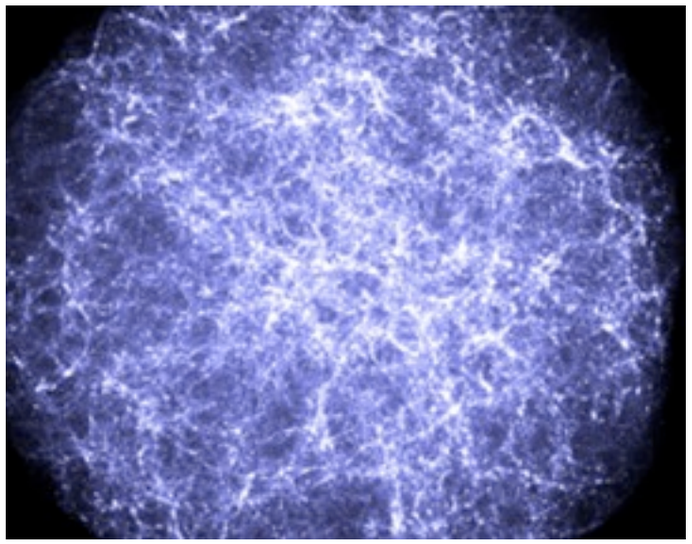
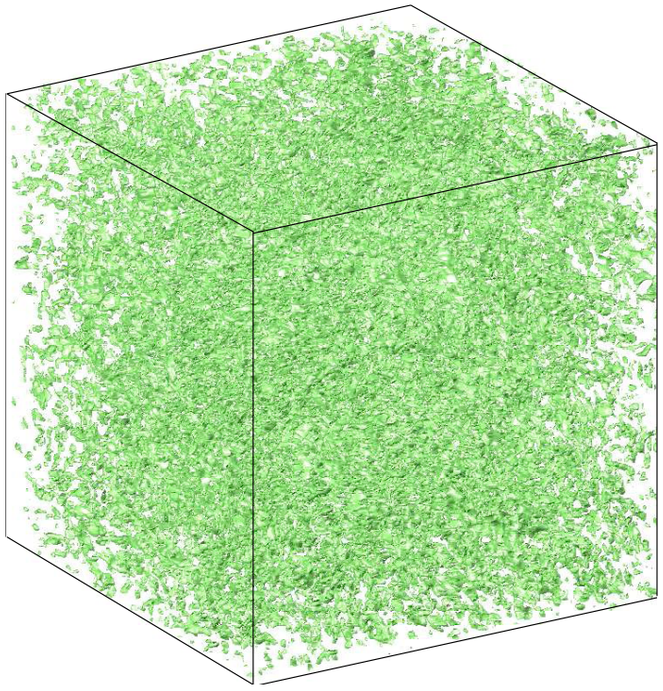
Previous Calculations

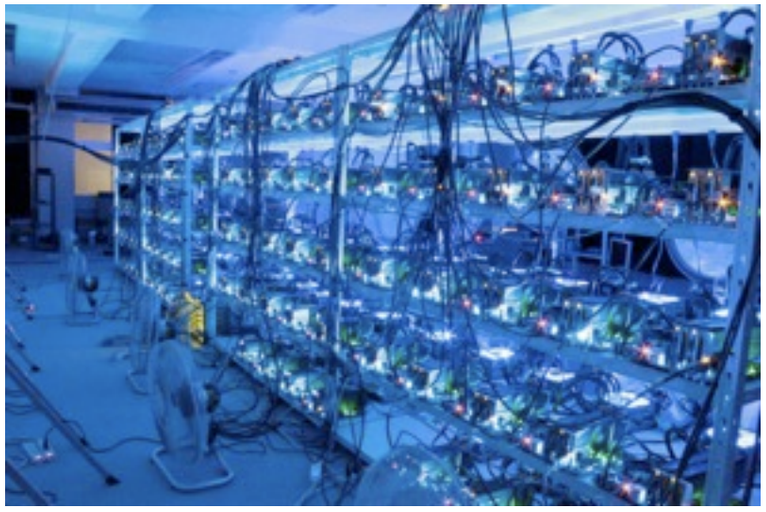


Astrophysics
Treecode
100 TFlops
N=3x10^9 : 6 sec
(Nitadori & Hamada)

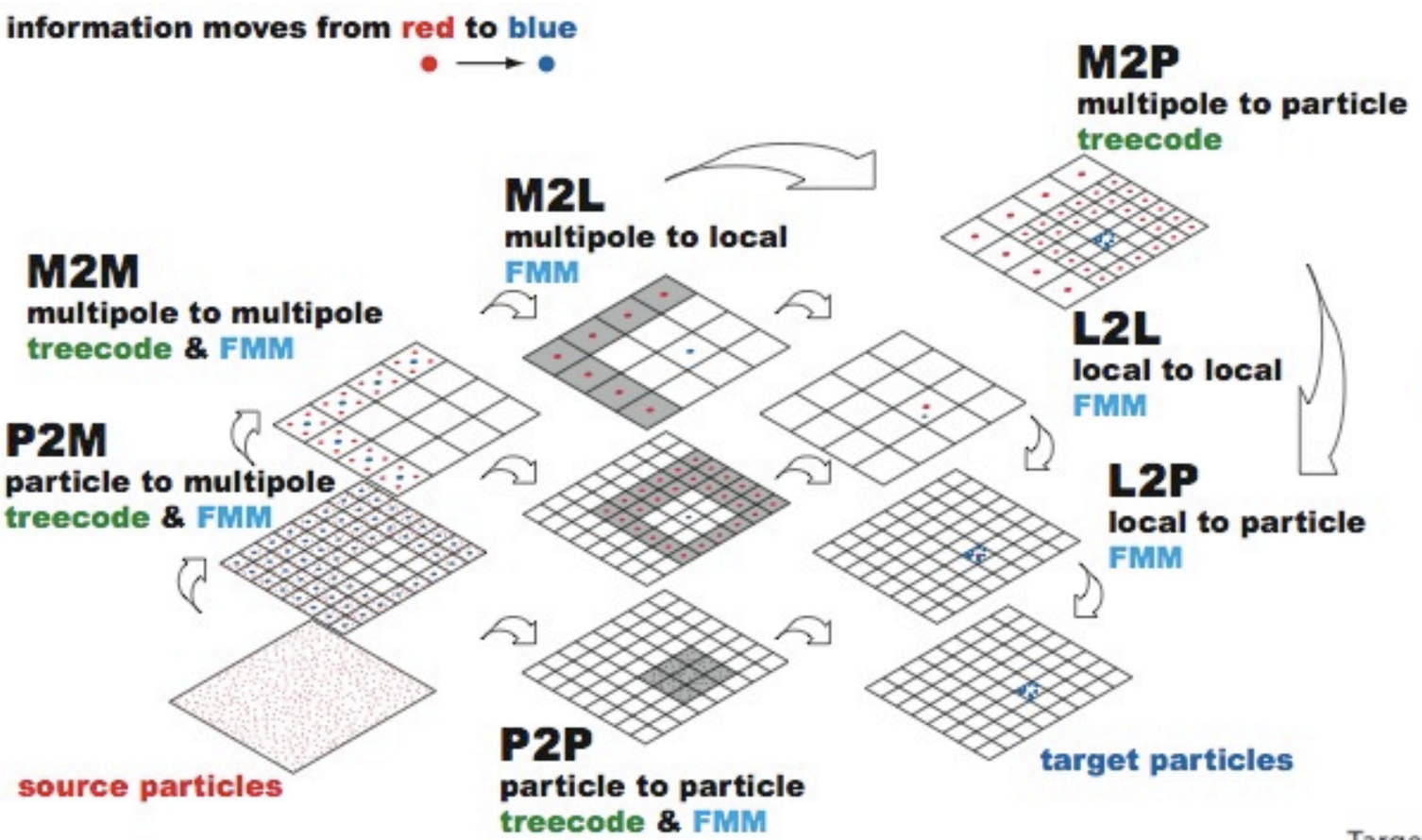


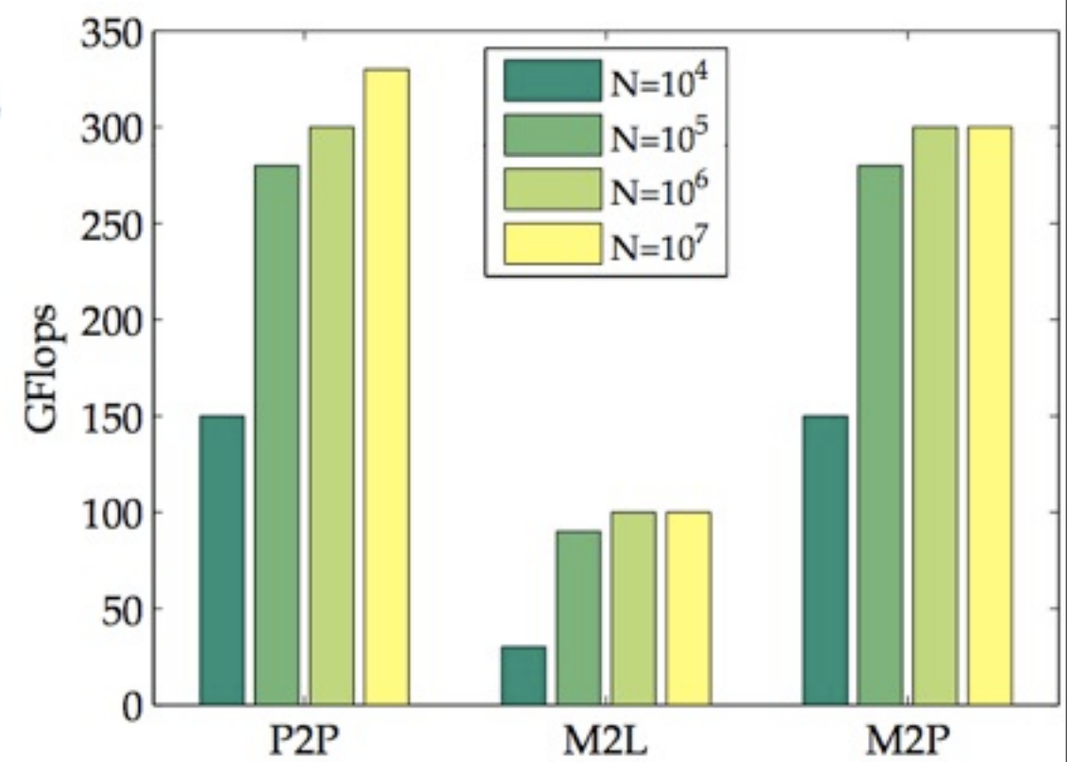
Turbulence
FMM
40 TFlops
N=3x10^9 : 20 sec
(Yokota & Barba)

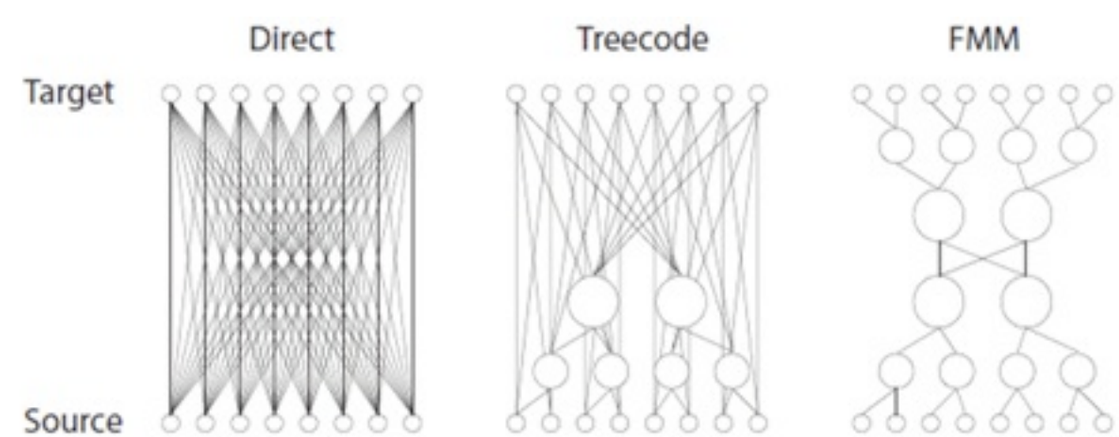
Nagasaki University
DEGIMA cluster
GTX295 x 380 = 760 GPUs
Theoretical Peak : 700 TFlops
Power Consumption : 100 kW



Treecode & FMM







Multipole expansion

$$\frac{1}{x_i - x_j} = \frac{1}{x_i - x_*} \frac{1}{\left(1 - \frac{x_j - x_*}{x_i - x_*}\right)}$$

and Taylor expansion

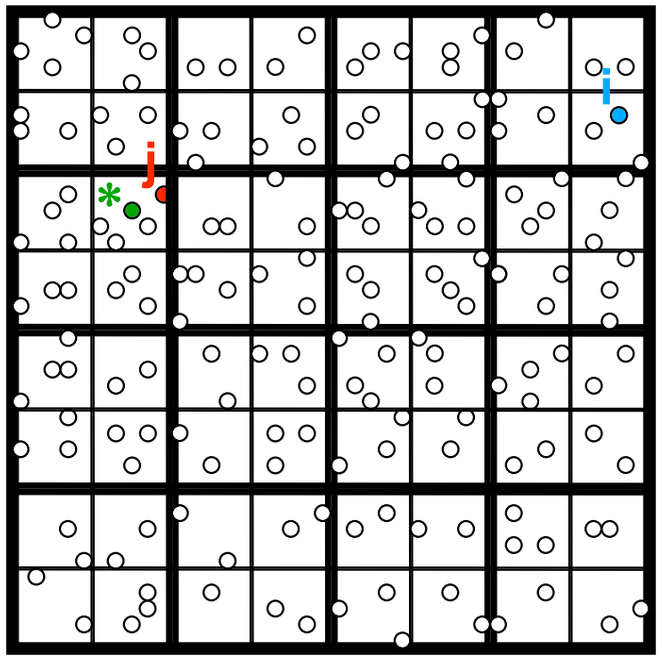
$$\frac{1}{1-t} = \sum_{k=0}^{p-1} t^k$$

gives

$$\sum_{j=1}^{N} \frac{1}{x_i - x_j}$$

$$= \sum_{j=1}^{N} \frac{1}{x_i - x_*} \left\{ \sum_{k=0}^{p-1} \left(\frac{x_j - x_*}{x_i - x_*} \right)^k \right\}$$

$$= \sum_{k=0}^{p-1} (x_i - x_*)^{-k-1} \left\{ \sum_{j=1}^{N} (x_j - x_*)^k \right\}$$

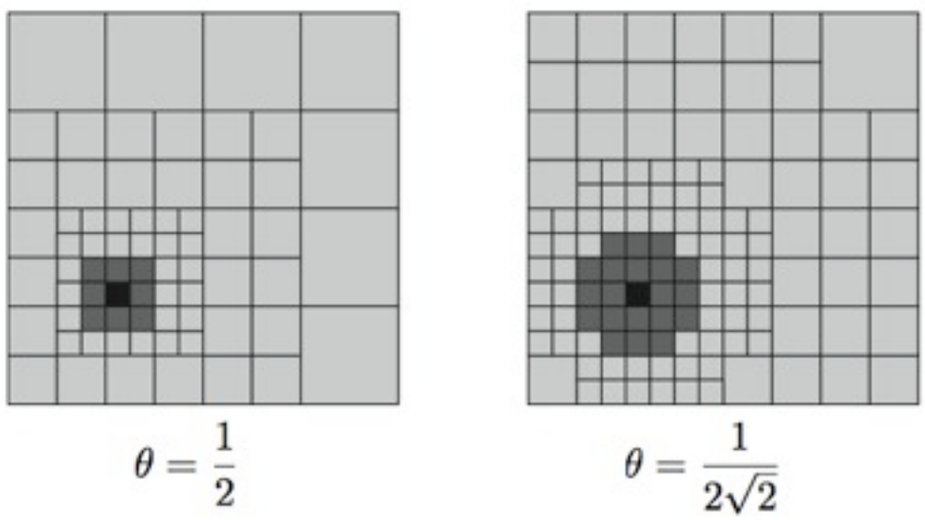


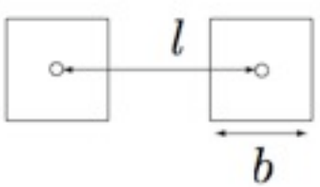

```
do i = 1,N
  ff = 0
  do j = 1,N
    ff = ff+1/ ( x( i )-x( j ) )
  end do
  f( i ) = ff
end do
```

```
do k = 1,p
  gg = 0
  do j = 1,N
    gg = gg+( x( j ) - xs )**( k-1 )
  end do
  g(k) = gg
end do
do i = 1,N
  ff = 0
  do k = 1,p
    ff = ff+( x( i )-xs )**( -k )*g( k-1 )
  end do
end do
```

Error Control

Treecode





$$\theta = \frac{b}{l}$$

FMM

$$\sum_{k=0}^{p-1}(x_i - x_*)^{-k-1}\left\{\sum_{j=1}^{N}(x_j - x_*)^k\right\}$$

Complexity	Error
$\mathcal{O}(p^3\theta^{-3})$	$\mathcal{O}(\theta^p)$

Error Optimization

Corrected Article: "An error-controlled fast multipole method" [J. Chem. Phys. 131, 244102 (2009)]

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Optimize p

Journal of Computational Physics **179,** 27–42 (2002)
doi:10.1006/jcph.2002.7026

A Hierarchical $\mathcal{O}(N)$ Force Calculation Algorithm

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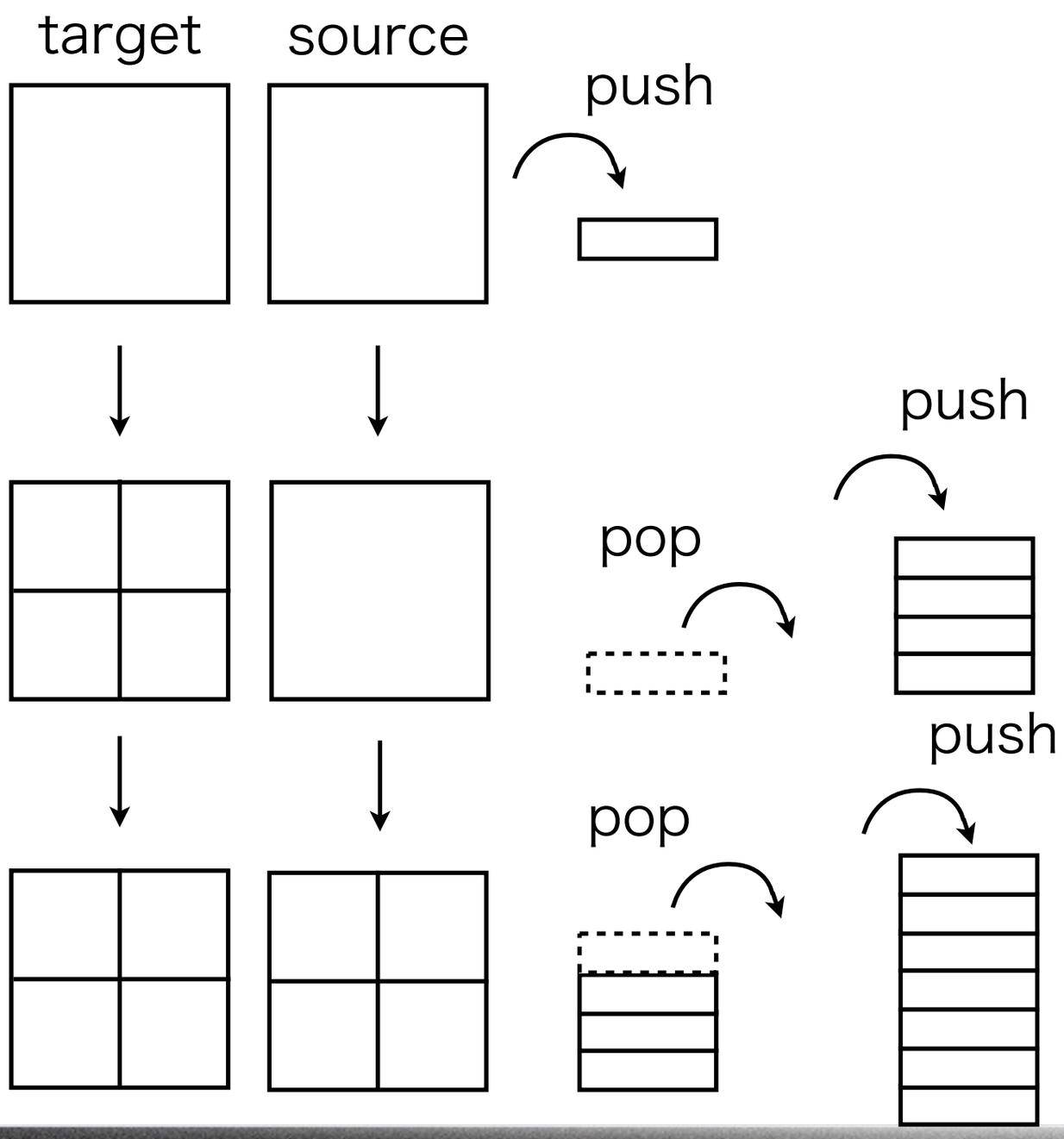
Optimize θ

↓

Better on GPUs?

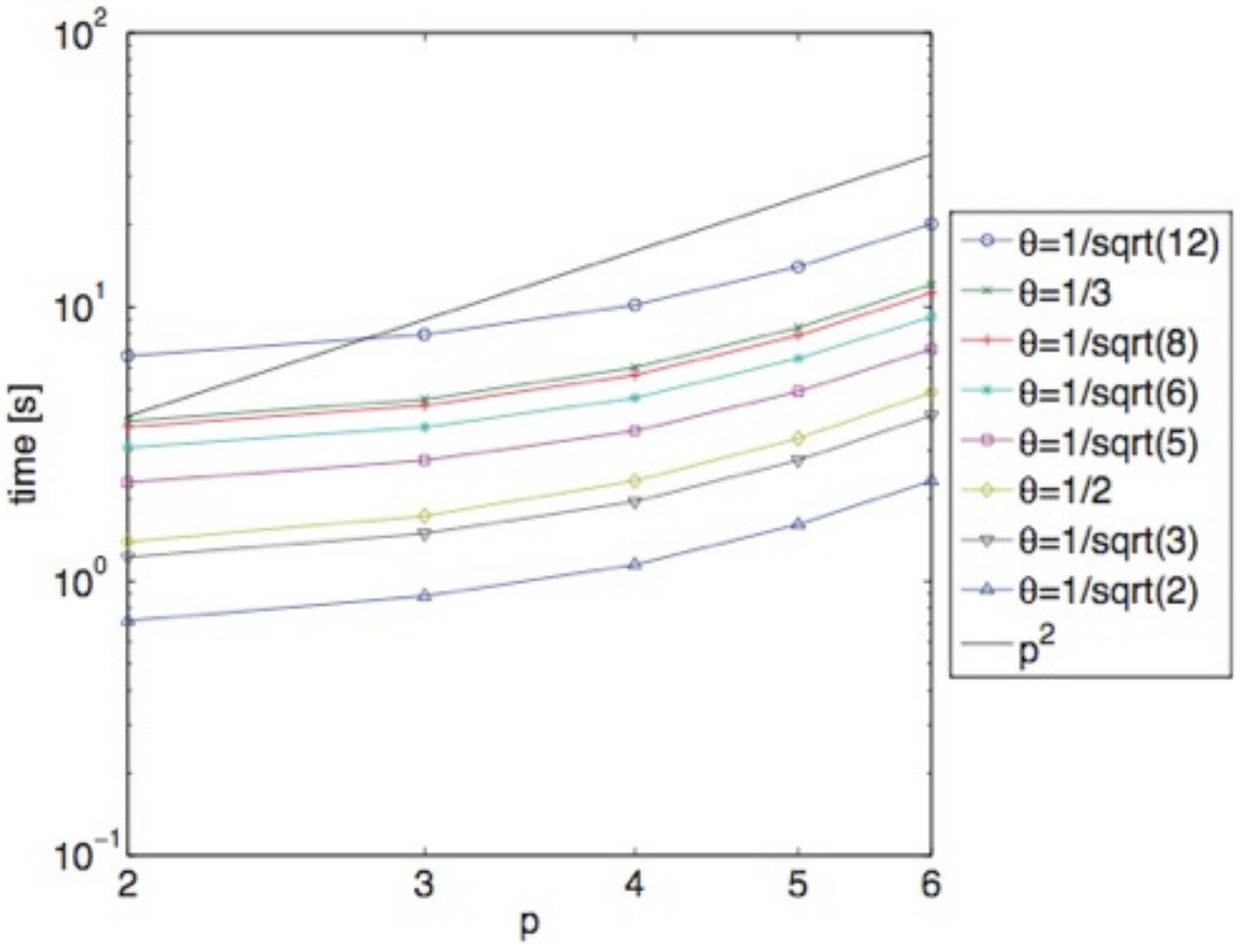
Stack based hybrid treewalk

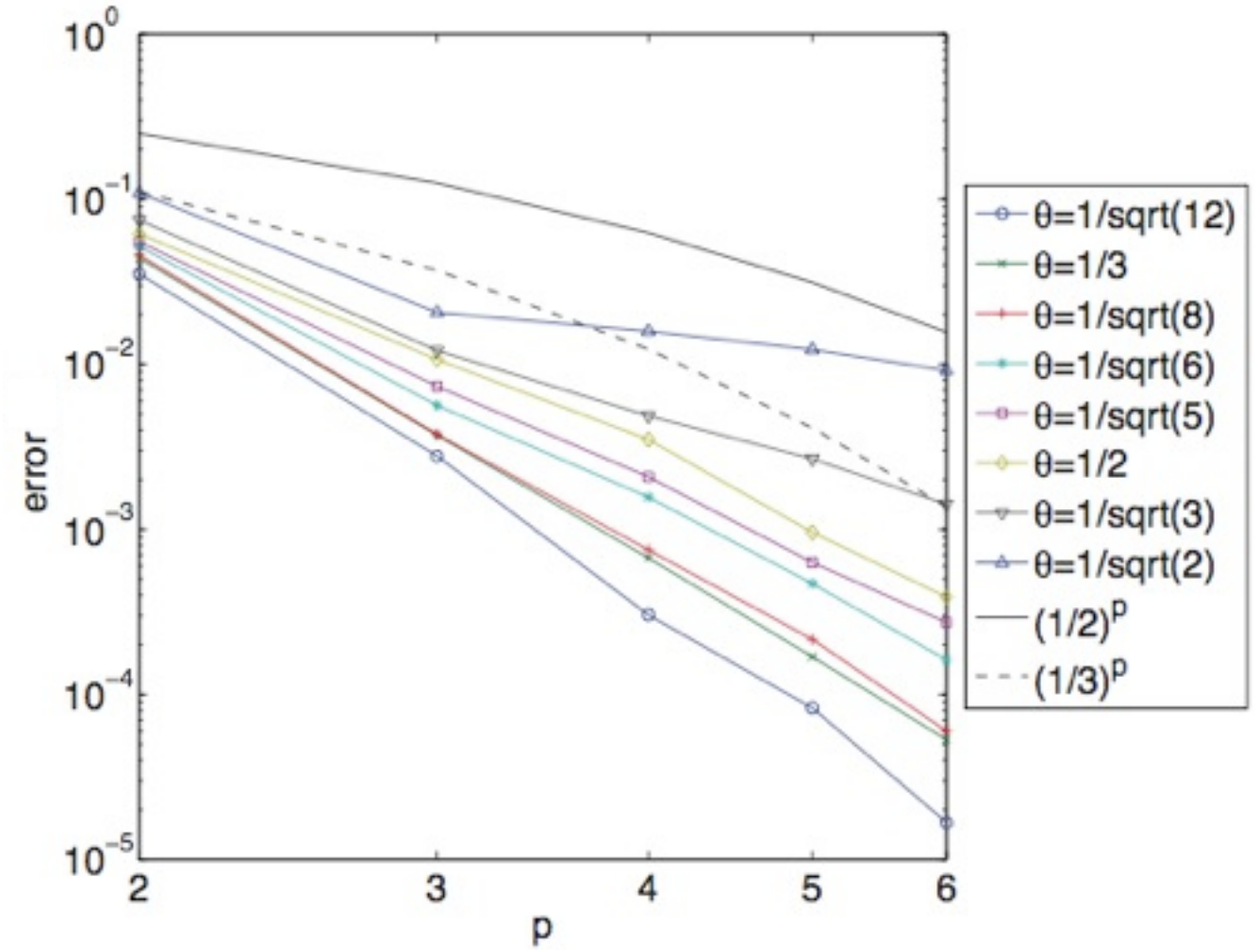


Algorithm Interact(cell A, cell B)

if there are very few particles in both cells, or they don't have child cells **then**
  Evaluate particle-particle (P2P)
else if cells A and B are well separated **then**
  if there are very few particles in cell A, or there are no child cells in cell A **then**
    Evaluate multipole-particle (M2P)
  else
    Evaluate multipole-local (M2L)
  end if
else
  Push pair(A,B) into a stack
end if

Parameter study





Complexity

$\mathcal{O}(p^3\theta^{-3})$

Error

$\mathcal{O}(\theta^p)$

Optimum parameters

Table 1: Calculation time of FMM on Xeon E5420 2.5GHz.

	P=2	P=3	P=4	P=5	P=6
$\theta = 1/\sqrt{12}$	6.6429	7.9396	10.1837	14.0261	20.1087
$\theta = 1/\sqrt{9}$	3.8470	4.6060	6.0223	8.4149	12.0948
$\theta = 1/\sqrt{8}$	3.6582	4.3763	5.6531	7.8727	11.2525
$\theta = 1/\sqrt{6}$	3.0775	3.6488	4.6646	6.4984	9.2089
$\theta = 1/\sqrt{5}$	2.2913	2.7581	3.5350	4.9221	7.0373
$\theta = 1/\sqrt{4}$	1.3953	1.7298	2.3248	3.3189	4.8830
$\theta = 1/\sqrt{3}$	1.2244	1.4930	1.9529	2.7644	4.0196
$\theta = 1/\sqrt{2}$	0.7172	0.8829	1.1484	1.6107	2.3244

Table 3: Calculation time of FMM on Tesla C1060.

	P=2	P=3	P=4	P=5	P=6
$\theta = 1/\sqrt{12}$	0.1441	0.1563	0.1662	0.1815	0.2022
$\theta = 1/\sqrt{9}$	0.1044	0.1106	0.1205	0.1318	0.1478
$\theta = 1/\sqrt{8}$	0.0991	0.1062	0.1162	0.1258	0.1400
$\theta = 1/\sqrt{6}$	0.0817	0.0859	0.0951	0.1061	0.1178
$\theta = 1/\sqrt{5}$	0.0662	0.0720	0.0778	0.0886	0.0979
$\theta = 1/\sqrt{4}$	0.0602	0.0668	0.0724	0.0804	0.0921
$\theta = 1/\sqrt{3}$	0.0573	0.0601	0.0660	0.0744	0.0822
$\theta = 1/\sqrt{2}$	0.0459	0.0482	0.0518	0.0576	0.0713

Table 2: $|L|^2$ error of FMM on Xeon E5420 2.5GHz.

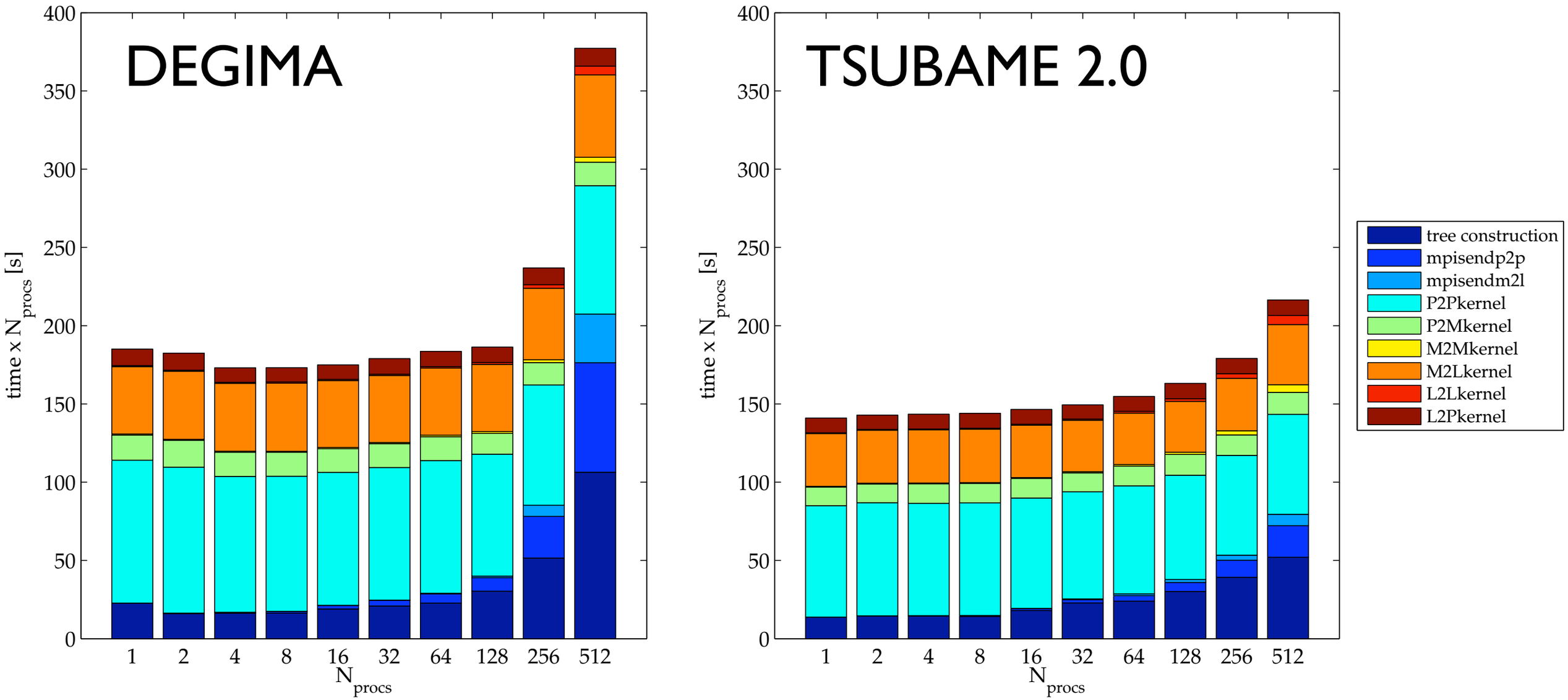
	P=2	P=3	P=4	P=5	P=6
$\theta = 1/\sqrt{12}$	3.5E-02	2.8E-03	3.0E-04	8.3E-05	1.7E-05
$\theta = 1/\sqrt{9}$	4.4E-02	3.7E-03	6.7E-04	1.7E-04	5.3E-05
$\theta = 1/\sqrt{8}$	4.6E-02	3.8E-03	7.5E-04	2.2E-04	6.0E-05
$\theta = 1/\sqrt{6}$	5.2E-02	5.6E-03	1.6E-03	4.7E-04	1.6E-04
$\theta = 1/\sqrt{5}$	5.5E-02	7.3E-03	2.1E-03	6.3E-04	2.7E-04
$\theta = 1/\sqrt{4}$	6.2E-02	1.1E-02	3.5E-03	9.6E-04	3.9E-04
$\theta = 1/\sqrt{3}$	7.5E-02	1.2E-02	4.9E-03	2.7E-03	1.4E-03
$\theta = 1/\sqrt{2}$	1.1E-01	2.1E-02	1.6E-02	1.2E-02	9.2E-03

Parallel calculation

Nagasaki University
DEGIMA
760 GTX295 GPUs
Peak : 0.7 PFlops

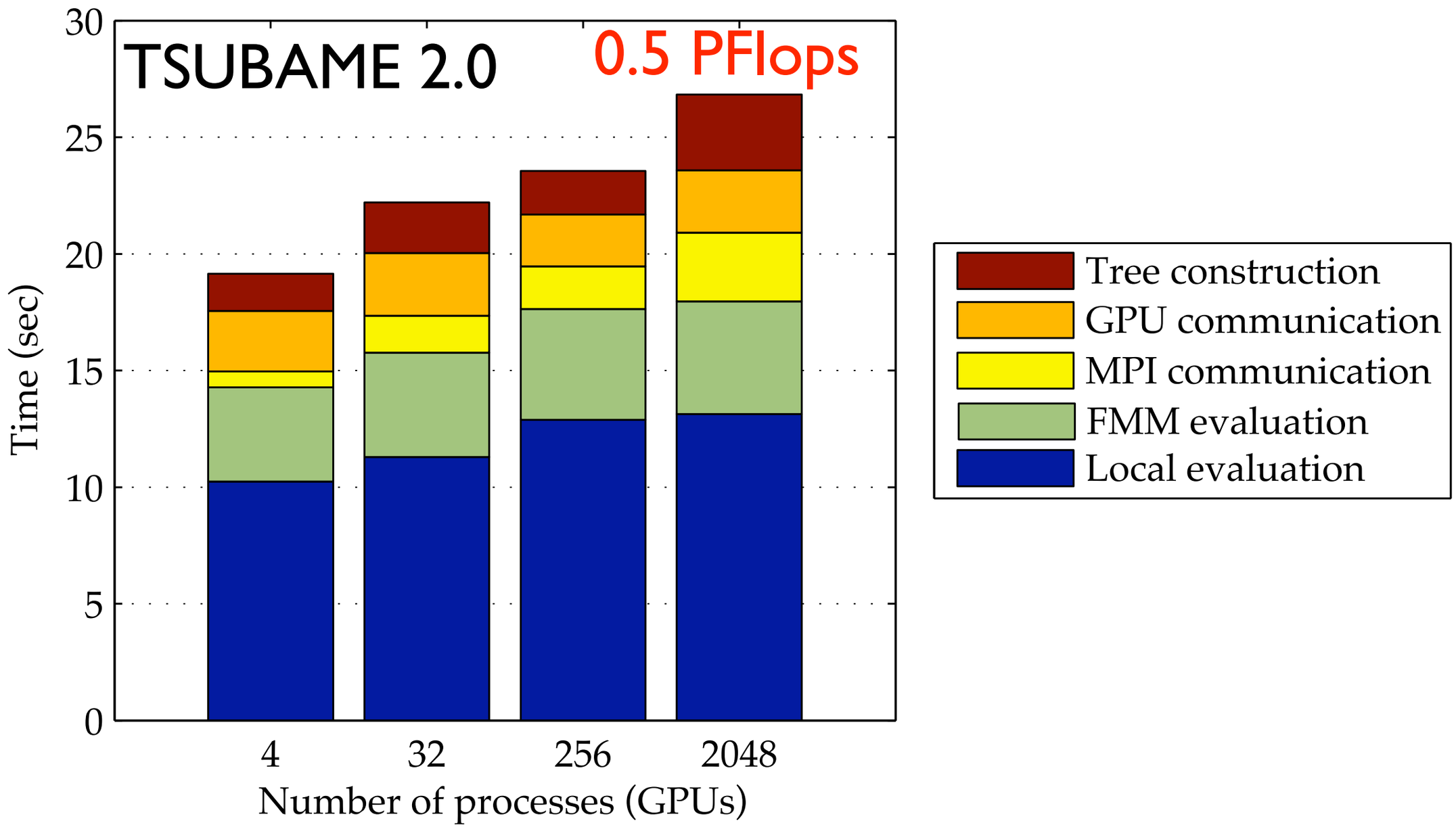
Tokyo Institute of Technology
TSUBAME 2.0
4224 M2050 GPUs
Peak : 2.4 PFlops

Strong Scaling



$N=10^8$

Weak Scaling



Summary & Outlook

1. The stack based treewalk enables a simple but effective hybridization of treecodes and FMMs

2. The optimum p and θ are different on CPUs and GPUs, but this difference is small

3. More tests need to be performed in the higher accuracy range and the overall performance must be compared to other treecodes and FMMs