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# Pipelining the Fast Multipole Method over a Runtime System

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Eric Darve<sup>b</sup>, Matthias Messner<sup>a</sup>, Toru Takahashi<sup>c</sup>

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# Outline

- ▶ Overview of the FMM
- ▶ FMM on a runtime system
- ▶ Results and performance analysis
- ▶ Conclusion and Perspectives

# Chebyshev Fast Multipole Method Overview

## N-body problems

Example, interactions between planets in a galaxy:



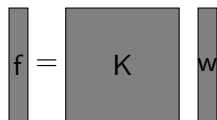
$N(N - 1)$  interactions  $\rightarrow$  **Complexity is  $O(N^2)$ .**

- ▶ Potentials (Kernel  $\approx 1/r$ )
  - ▶ Electrostatic  $\rightarrow$  Molecular dynamics
  - ▶ Gravitational  $\rightarrow$  Astrophysics
  - ▶ but also electromagnetism, fluid dynamics, VLSI capacitance,  
...

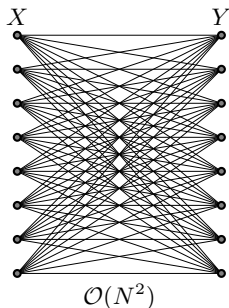
## FMM : Motivations

- ▶ Pairwise interactions among  $N$  bodies.

$$f_i = \sum_{j=1}^N K(x_i, x_j) w_j \quad \text{for } i = 1, \dots, N.$$



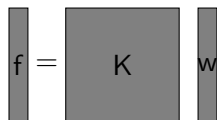
- ▶ **Direct computation**  $\mathcal{O}(N^2)$



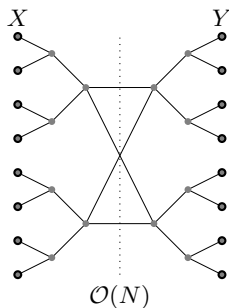
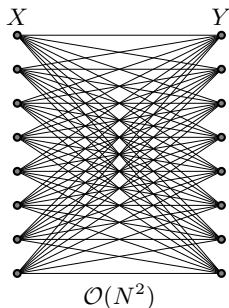
## FMM : Motivations

- Pairwise interactions among  $N$  bodies.

$$f_i = \sum_{j=1}^N K(x_i, x_j) w_j \quad \text{for } i = 1, \dots, N.$$



- Direct computation**  $O(N^2)$   $\rightarrow$  **FMM**  $O(N)$ .

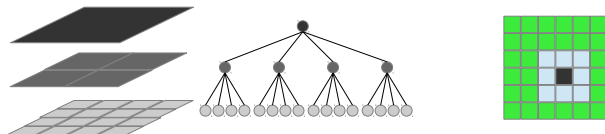


# FMM : Overview

- ▶ Potential decomposition

$$f_i = f_i^{near} + f_i^{far}$$

- ▶ Involve hierarchical space decomposition with a tree (**octree**)



- ▶ **Near field** is computed by direct interactions.
- ▶ Different approaches to approximate the **far field**
  - ▶ Expansions (Cartesian or Spherical)
  - ▶ **Interpolation** (Chebyshev FMM)



## Chebyshev FMM

Idea: Interpolate the kernel on a Chebyshev grid

$$\frac{1}{|\mathbf{x} - \mathbf{y}|} \sim \sum_{m=1}^{\ell} S_{\ell}(\mathbf{x}, \bar{x}_m) \sum_{n=1}^{\ell} \frac{1}{|\bar{x}_m - \bar{y}_n|} S_{\ell}(\mathbf{y}, \bar{y}_n)$$

## Chebyshev FMM

Idea: Interpolate the kernel on a Chebyshev grid

$$\frac{1}{|\mathbf{x} - \mathbf{y}|} \sim \sum_{m=1}^{\ell} S_{\ell}(\mathbf{x}, \bar{x}_m) \sum_{n=1}^{\ell} \frac{1}{|\bar{x}_m - \bar{y}_n|} S_{\ell}(\mathbf{y}, \bar{y}_n)$$

$S_{\ell}$  is the interpolation polynomial (the higher  $\ell$  the more accurate is the far field)

$$S_{\ell}(x, x_m) = \frac{1}{\ell} + \frac{2}{\ell} \sum_{n=1}^{\ell-1} T_n(\bar{x}_m) T_n(x)$$

## Chebyshev FMM

Idea: Interpolate the kernel on a Chebyshev grid

$$\frac{1}{|\mathbf{x} - \mathbf{y}|} \sim \sum_{m=1}^{\ell} S_{\ell}(\mathbf{x}, \bar{x}_m) \sum_{n=1}^{\ell} \frac{1}{|\bar{x}_m - \bar{y}_n|} S_{\ell}(\mathbf{y}, \bar{y}_n)$$

$S_{\ell}$  is the interpolation polynomial (the higher  $\ell$  the more accurate is the far field)

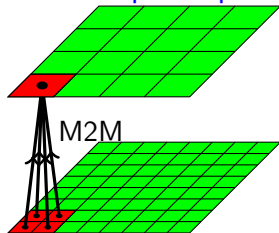
$$S_{\ell}(x, x_m) = \frac{1}{\ell} + \frac{2}{\ell} \sum_{n=1}^{\ell-1} T_n(\bar{x}_m) T_n(x)$$

For all  $i = 1, \dots, N$ .

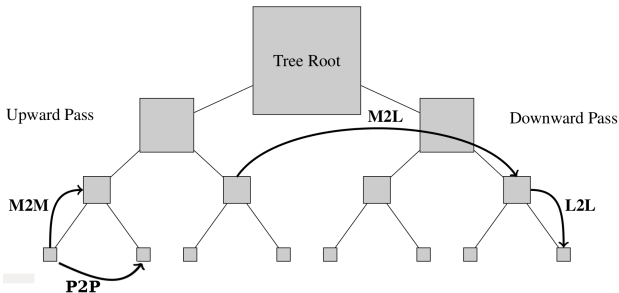
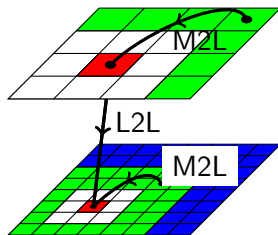
$$f_i = \sum_{j=1}^N \frac{1}{|x_i - y_j|} w_j$$
$$\sim \underbrace{\sum_{m=1}^{\ell} S_{\ell}(x_i, \bar{x}_m)}_{\text{L2L}} \underbrace{\sum_{n=1}^{\ell} \frac{1}{|\bar{x}_m - \bar{y}_n|}}_{\text{M2L}} \underbrace{\sum_{j=1}^{N^{far}} S_{\ell}(y_j, \bar{y}_n)}_{\text{M2M}} w_j + \underbrace{\sum_{j=1}^{N^{near}} \frac{1}{|x_i - y_j|} w_j}_{\text{P2P}}$$

# FMM : $O(N)$ algorithm

Upward pass



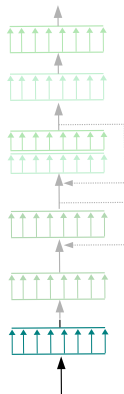
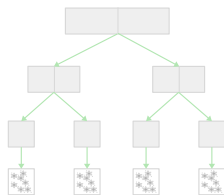
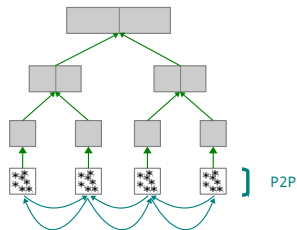
Downward pass



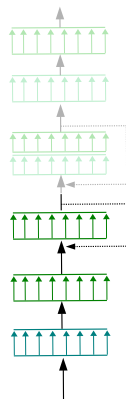
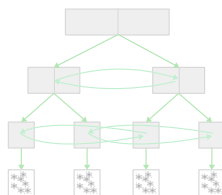
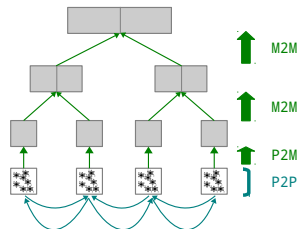
# FMM on a runtime



# Fork-join parallelization : Simplified illustration

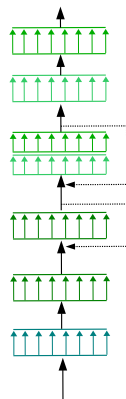
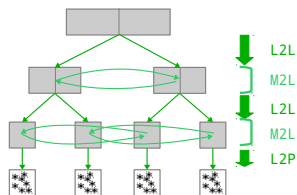
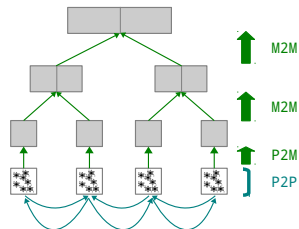


# Fork-join parallelization : Simplified illustration

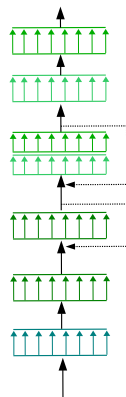
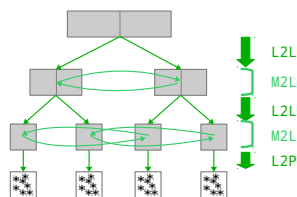
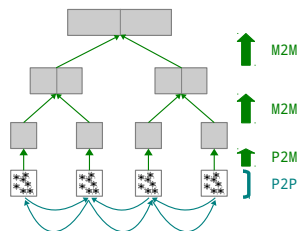




# Fork-join parallelization : Simplified illustration

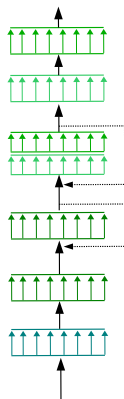
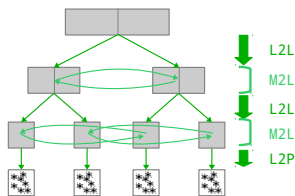
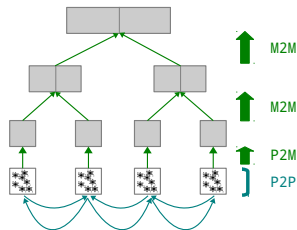


## Fork-join parallelization : Simplified illustration

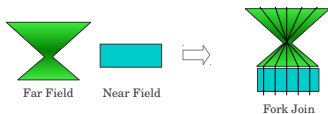


Limits: Synchronizations (+ bottleneck at the top of the tree).

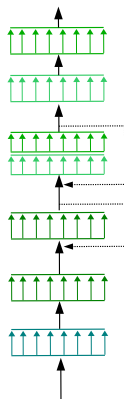
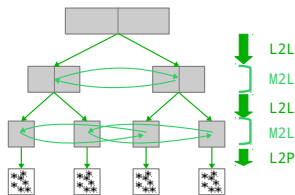
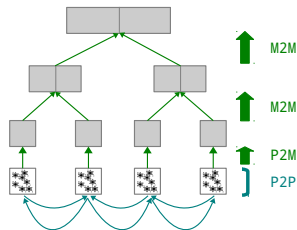
# Fork-join parallelization : Simplified illustration



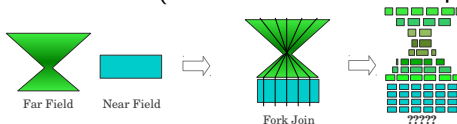
Limits: Synchronizations (+ bottleneck at the top of the tree).



# Fork-join parallelization : Simplified illustration



Limits: Synchronizations (+ bottleneck at the top of the tree).



# StarPU : Description

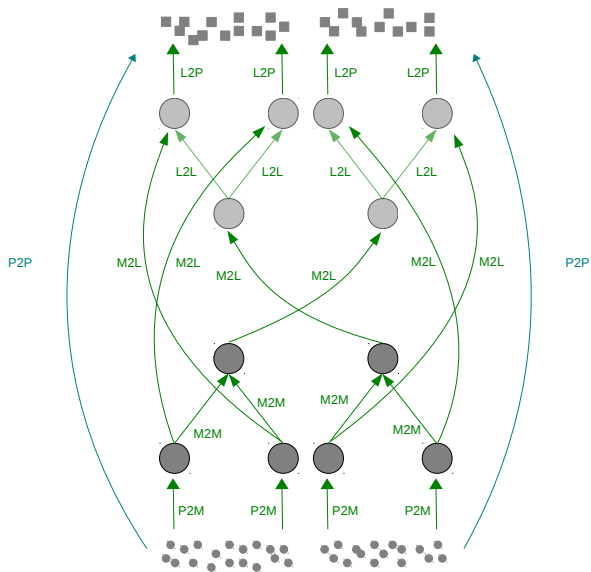
## StarPU runtime

- ▶ Advanced tasks scheduling (customizable scheduler)
- ▶ Tasks dependencies expression
- ▶ Gives an abstraction of the architecture (useful for accelerators)
- ▶ <http://runtime.bordeaux.inria.fr/StarPU/>

## Insert\_task function:

- ▶ `insert_task` ( operator, {READ,WRITE}, data, ... )

# Exploiting the parallelism of the FMM



# StarPU : Simplified example

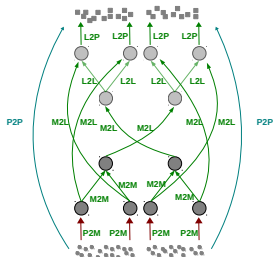
Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
```

```
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
```

```
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
```

```
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```



# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
```

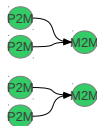
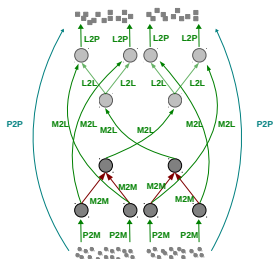
```
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
```

```
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
```

```
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
```

```
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```





# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
```

```
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
```

```
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
```

```
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
```

```
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[1][0].interaction, WRITE, cell[2][0])
```

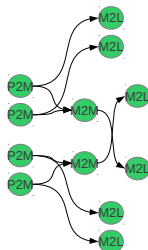
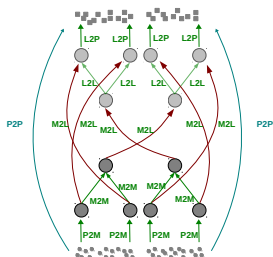
```
insert_task(M2L, READ, cell[1][1].interaction, WRITE, cell[2][1])
```

```
insert_task(M2L, READ, cell[2][0].interaction, WRITE, cell[2][0])
```

```
insert_task(M2L, READ, cell[2][1].interaction, WRITE, cell[2][1])
```

```
insert_task(M2L, READ, cell[2][2].interaction, WRITE, cell[2][2])
```

```
insert_task(M2L, READ, cell[2][3].interaction, WRITE, cell[2][3])
```



# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
```

```
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
```

```
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
```

```
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
```

```
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[1][0].interaction, WRITE, cell[2][0])
```

```
insert_task(M2L, READ, cell[1][1].interaction, WRITE, cell[2][1])
```

```
insert_task(M2L, READ, cell[2][0].interaction, WRITE, cell[2][0])
```

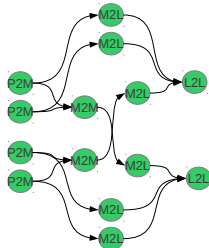
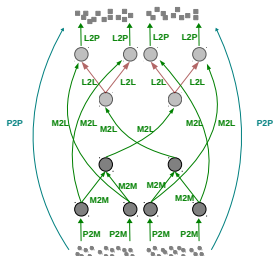
```
insert_task(M2L, READ, cell[2][1].interaction, WRITE, cell[2][1])
```

```
insert_task(M2L, READ, cell[2][2].interaction, WRITE, cell[2][2])
```

```
insert_task(M2L, READ, cell[2][3].interaction, WRITE, cell[2][3])
```

```
insert_task(L2L, READ, cell[1][0], WRITE, cell[2][0], cell[2][1])
```

```
insert_task(L2L, READ, cell[1][1], WRITE, cell[2][2], cell[2][3])
```



# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

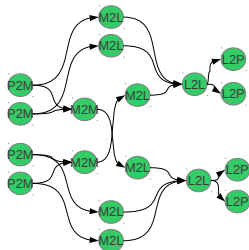
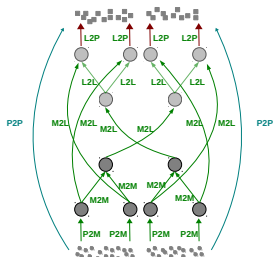
```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[1][0].interaction, WRITE, cell[1][0])
insert_task(M2L, READ, cell[1][1].interaction, WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[2][0].interaction, WRITE, cell[2][0])
insert_task(M2L, READ, cell[2][1].interaction, WRITE, cell[2][1])
insert_task(M2L, READ, cell[2][2].interaction, WRITE, cell[2][2])
insert_task(M2L, READ, cell[2][3].interaction, WRITE, cell[2][3])
```

```
insert_task(L2L, READ, cell[1][0], WRITE, cell[2][0], cell[2][1])
insert_task(L2L, READ, cell[1][1], WRITE, cell[2][2], cell[2][3])
```

```
insert_task(L2P, READ, cell[2][0], WRITE, particles[0])
insert_task(L2P, READ, cell[2][1], WRITE, particles[1])
insert_task(L2P, READ, cell[2][2], WRITE, particles[2])
insert_task(L2P, READ, cell[2][3], WRITE, particles[3])
```



# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```

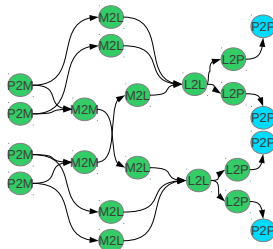
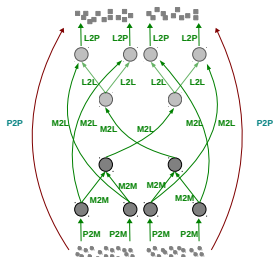
```
insert_task(M2L, READ, cell[1][0].interaction, WRITE, cell[1][0])
insert_task(M2L, READ, cell[1][1].interaction, WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[2][0].interaction, WRITE, cell[2][0])
insert_task(M2L, READ, cell[2][1].interaction, WRITE, cell[2][1])
insert_task(M2L, READ, cell[2][2].interaction, WRITE, cell[2][2])
insert_task(M2L, READ, cell[2][3].interaction, WRITE, cell[2][3])
```

```
insert_task(L2L, READ, cell[1][0], WRITE, cell[2][0], cell[2][1])
insert_task(L2L, READ, cell[1][1], WRITE, cell[2][2], cell[2][3])
```

```
insert_task(L2P, READ, cell[2][0], WRITE, particles[0])
insert_task(L2P, READ, cell[2][1], WRITE, particles[1])
insert_task(L2P, READ, cell[2][2], WRITE, particles[2])
insert_task(L2P, READ, cell[2][3], WRITE, particles[3])
```

```
insert_task(P2P, READ, neighbours[0], WRITE, particles[0])
insert_task(P2P, READ, neighbours[1], WRITE, particles[1])
insert_task(P2P, READ, neighbours[2], WRITE, particles[2])
insert_task(P2P, READ, neighbours[3], WRITE, particles[3])
```



# StarPU : Simplified example

Cells access  $\rightarrow$  cell[level][position]

```
insert_task(P2M, READ, particles[0], WRITE, cell[2][0])
```

```
insert_task(P2M, READ, particles[1], WRITE, cell[2][1])
```

```
insert_task(P2M, READ, particles[2], WRITE, cell[2][2])
```

```
insert_task(P2M, READ, particles[3], WRITE, cell[2][3])
```

```
insert_task(M2M, READ, cell[2][0], cell[2][1], WRITE, cell[1][0])
```

```
insert_task(M2M, READ, cell[2][2], cell[2][3], WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[1][0].interaction, WRITE, cell[1][0])
```

```
insert_task(M2L, READ, cell[1][1].interaction, WRITE, cell[1][1])
```

```
insert_task(M2L, READ, cell[2][0].interaction, WRITE, cell[2][0])
```

```
insert_task(M2L, READ, cell[2][1].interaction, WRITE, cell[2][1])
```

```
insert_task(M2L, READ, cell[2][2].interaction, WRITE, cell[2][2])
```

```
insert_task(M2L, READ, cell[2][3].interaction, WRITE, cell[2][3])
```

```
insert_task(L2L, READ, cell[1][0], WRITE, cell[2][0], cell[2][1])
```

```
insert_task(L2L, READ, cell[1][1], WRITE, cell[2][2], cell[2][3])
```

```
insert_task(P2P, READ, neighbours[0], WRITE, particles[0])
```

```
insert_task(P2P, READ, neighbours[1], WRITE, particles[1])
```

```
insert_task(P2P, READ, neighbours[2], WRITE, particles[2])
```

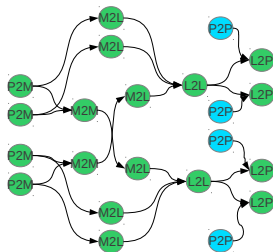
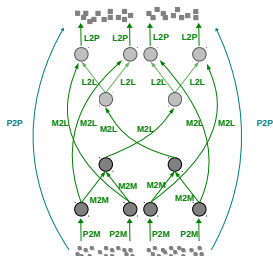
```
insert_task(P2P, READ, neighbours[3], WRITE, particles[3])
```

```
insert_task(L2P, READ, cell[2][0], WRITE, particles[0])
```

```
insert_task(L2P, READ, cell[2][1], WRITE, particles[1])
```

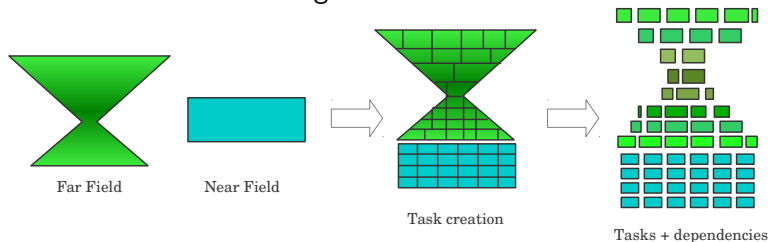
```
insert_task(L2P, READ, cell[2][2], WRITE, particles[2])
```

```
insert_task(L2P, READ, cell[2][3], WRITE, particles[3])
```



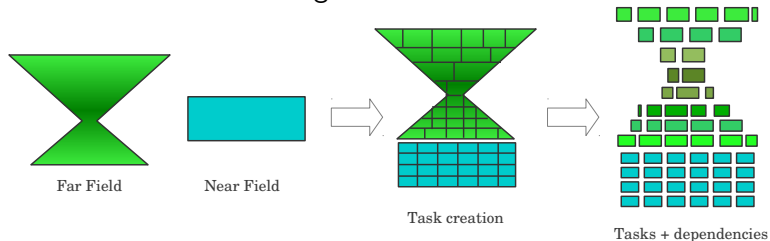
# StarPU : Tasks creation and execution

Creation of the tasks using insert function:

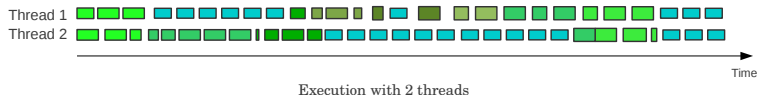


# StarPU : Tasks creation and execution

Creation of the tasks using insert function:



Execution of the tasks (trace):



# StarPU : Using GPU kernels

Two GPU kernels : P2P and M2L

- ▶ P2P & M2L represent more than 90% of the work

Scheduling:

- ▶ Schedulers assign tasks to processing units.
- ▶ StarPU proposes several schedulers (but none fits our needs).
- ▶ We developed a new scheduler:
  - ▶ Based on Eager
  - ▶ Enable setting priorities to operators
  - ▶ Different priorities for GPU or CPU



# Results & Performance

# Experimental Setup

## ScalFMM:

- ▶ Developed in C++ (OpenMP, MPI, and now StarPU)
- ▶ Available at <http://scalfmm-public.gforge.inria.fr/>

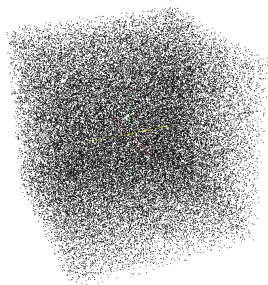
## Test cluster:

- ▶ Heterogeneous 12 CPU and 3 GPU
- ▶ CPU dual-socket hexa-core Intel X5650 Nehalem (2.67 GHz)
- ▶ GPU Nvidia M2070 (or M2090)

In the following results Intel Compiler (12.0.5) is used.

## Test case

- ▶ Uniform distribution of particles in 3D inside a cube
- ▶ Particles  $30 \cdot 10^6$
- ▶ Granularity  $n_g = 2000$
- ▶ Octree height  $h = \{6, 7\}$
- ▶  $Acc(\ell) = 10^{-\ell}$ , with  $\ell = \{2 - 7\}$
- ▶  $GPU = \{0, 1, 2, 3\}$

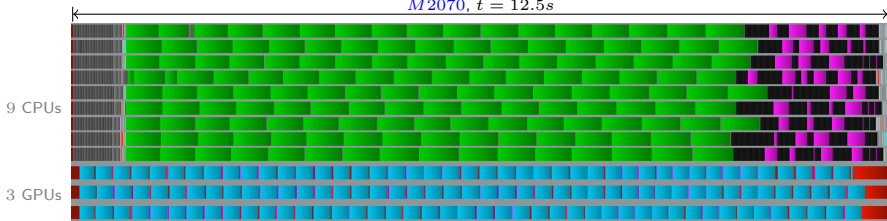


# StarPU Execution traces M2070-M2090

Particles  $30 \cdot 10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$ ,  
 $Acc(\ell = 5) = 10^{-5}$



M2070,  $t = 12.5s$



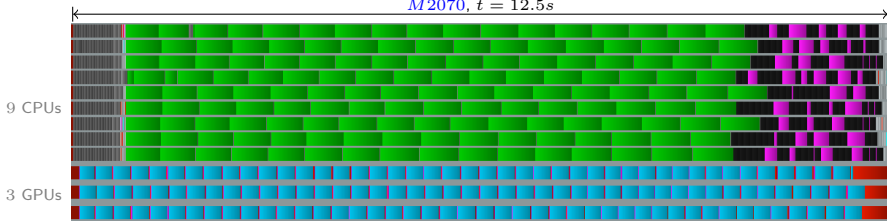
Legend : P2P, P2M, M2M, M2L, L2L, L2P, Idle, Moving data .

# StarPU Execution traces M2070-M2090

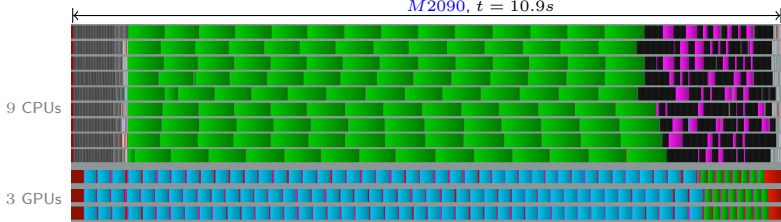
Particles  $30.10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$ ,  
 $Acc(\ell = 5) = 10^{-5}$



*M2070*,  $t = 12.5s$



*M2090*,  $t = 10.9s$



Legend : P2P, P2M, M2M, M2L, L2L, L2P, Idle, Moving data .

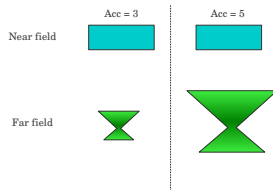
# StarPU Execution traces M2070

Particles  $30 \cdot 10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$



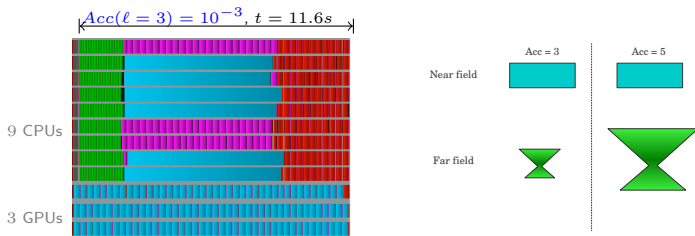
# StarPU Execution traces M2070

Particles  $30.10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$



# StarPU Execution traces M2070

Particles  $30 \cdot 10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$

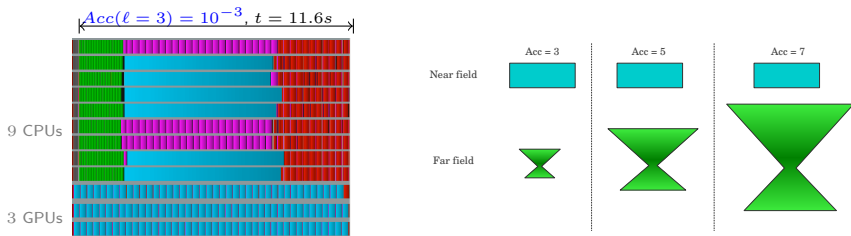


Legend : P2P, P2M, M2M, M2L, L2L, L2P, Idle, Moving data .



# StarPU Execution traces M2070

Particles  $30 \cdot 10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$

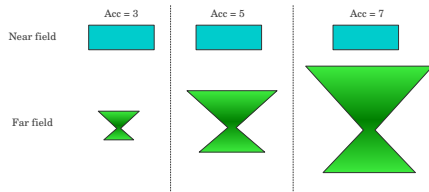
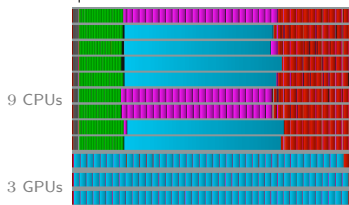


Legend : P2P, P2M, M2M, M2L, L2L, L2P, Idle, Moving data .

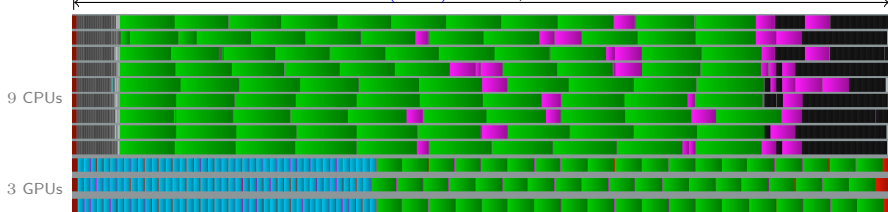
# StarPU Execution traces M2070

Particles  $30.10^6$ , Octree height  $h = 6$ , Granularity  $n_g = 2000$

$Acc(\ell = 3) = 10^{-3}$ ,  $t = 11.6s$



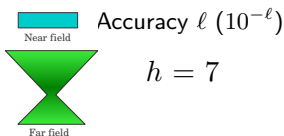
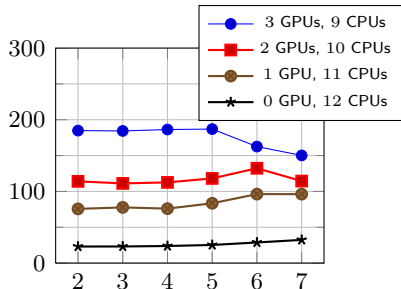
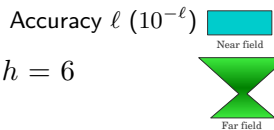
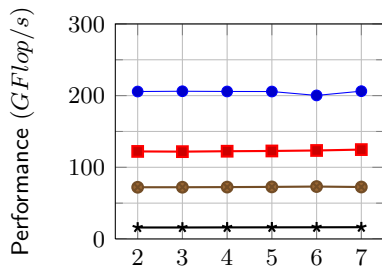
$Acc(\ell = 7) = 10^{-7}$ ,  $t = 33.5s$



Legend : P2P, P2M, M2M, M2L, L2L, L2P, Idle, Moving data .

# Results M2070

30.10<sup>6</sup> particles inside a box, granularity  $n_g = 2000$ , for 0 to 3 GPU and accuracy from 2 to 7.



## Conclusion

- ▶ Runtime optimization of parallel mapping was demonstrated.
- ▶ Modern heterogeneous computing platforms lead to hard DAG scheduling.
- ▶ Approach like Fork-join may be insufficient.
- ▶ Code is hardware “independent.” Schedulers determine the best processor to execute a given task.

## Acknowledgement

- ▶ Inria & FastLA associate team.
- ▶ StarPU development team.
- ▶ ScalFMM <http://scalfmm-public.gforge.inria.fr/>

Thanks - Questions?



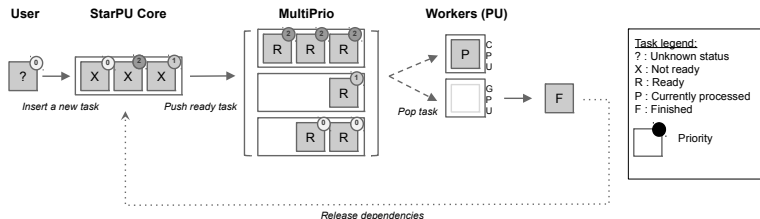
Annexes

Annexes

The logo for Inria, featuring the word "Inria" in a stylized, cursive font with a color gradient from red to orange. Above the "ria" part of the word, the words "informatics" and "mathematics" are written in a smaller, black, sans-serif font, separated by a small dot.

*Inria*  
informatics mathematics

# Annexe : Scheduler



## Annexe : Using CPU and GPU

---

---

```
function M2L()  
  forall the levels lv from 2 to leaf_level do  
    foreach Block bl in blocks[lv] do  
      insert_task( cpu_m2l, gpu_m2l, READ, bl.interactions,  
                  WRITE, bl);
```

---

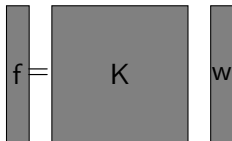
- ▶ StarPU is able to compute a M2L on the CPU or on the device (after moving the data)



## Chebyshev FMM : Direct Matrix Vector

▶  $f = K w$

▶  $(K)_{ij} = K(x_i, y_j) = \frac{1}{|x_i - y_j|}$

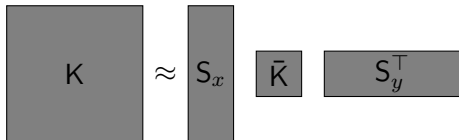


Interpolation based Matrix Vector (low rank approximation)

▶  $K \approx S_x \bar{K} S_y^T$

▶  $S_x, S_y \dim N \times \ell^3$

▶  $\bar{K} \dim \ell^3 \times \ell^3$



Second low rank approximation (SVD)

▶  $\bar{K} \approx U V^T$

▶  $U, V \dim \ell^3 \times r$

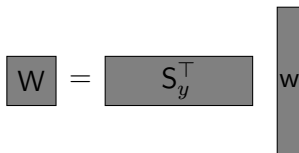


# Chebyshev FMM : Interpolation based Matrix Vector

$$f = K w \approx S_x \bar{K} S_y^T w$$

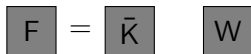
P2M/M2M:

▶  $W = S_y^T w$



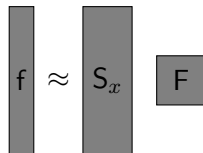
M2L:

▶  $F = \bar{K} W$



L2L/L2P:

▶  $f \approx S_x F$



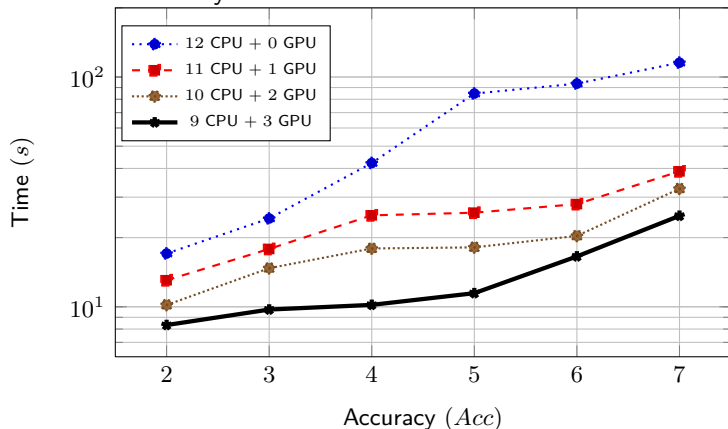
## Task : Introduction

A task is composed by:

- ▶ A block of instructions
- ▶ Some parameters
- ▶ An environment
- ▶ Tasks is native in many "libraries" (OpenMP 3.1, StarPU)

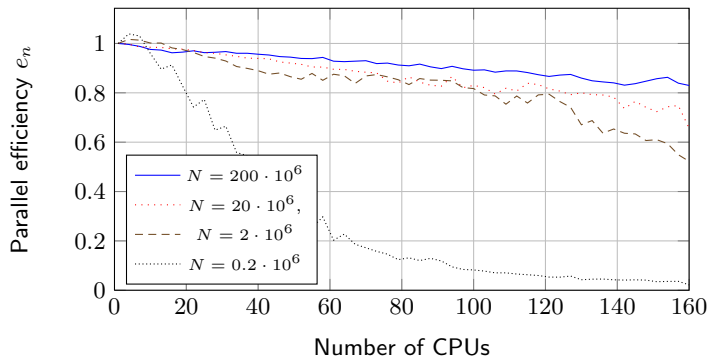
## Results M2070

$30 \cdot 10^6$  particles inside a box, granularity  $n_g = 2000$ , for 0 to 3 GPU and accuracy from 2 to 7.



## 160 Cores efficiency

$\{N = 0.2 \cdot 10^6, n_g = 25, h = 5\}$ ,  $\{N = 2 \cdot 10^6, n_g = 200, h = 6\}$   
 $\{N = 20 \cdot 10^6, n_g = 1000, h = 7\}$ ,  $\{N = 200 \cdot 10^6, n_g = 3000, h = 8\}$



# StarPU : Creating tasks

Examples:

---

---

```
insert_task(m2m, READ, children, WRITE, cell);
```

---

---

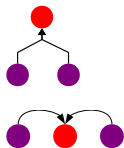
---

---

```
insert_task(m2l, READ, interactions, WRITE, cell);
```

---

---



Order of insertion matters:

- ▶ It leads to the DAG
- ▶ Different orders can create different DAG