3D Cartesian Transport Sweep for Massively Parallel Architectures on top of PaRSEC

9th Scheduling for Large Scale Systems Workshop, Lyon

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1
Context and goals

Guideline

Context

- EDF R&D is looking for a Fast Reference Solver
- PhD Student: Salli Moustafa

- Industrial solvers:
  - diffusion approximation ($\approx$ SP1);
  - COCAGNE (SPN).

- Solution on more than 10^{11} degrees of freedom (DoFs) involved
  - probabilistic solvers (very long computation time);
  - deterministic solvers.

DOMINO (SN) is designed for this validation purpose.

DOMINO: Discrete Ordinates Method In NeutrOnics

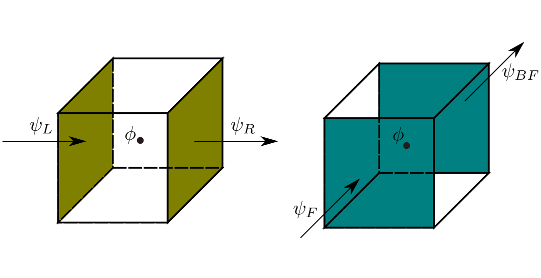
- Deterministic, Cartesian, and 3D solver;
- 3 levels of discretization:
  - energy (G): multigroup formalism;
  - angle ($\vec{\Omega}$): *Level Symmetric Quadrature*, $N(N+2)$ directions
  - space (x, y, z): *Diamond Differencing scheme* (order 0);
- 3 nested levels of iterations:
  - power iterations + Chebychev acceleration;
  - multigroup iterations: Gauss–Seidel algorithm;
  - scattering iterations + DSA acceleration (using the SPN solver):
    $\rightarrow$ spatial sweep, which consumes most of the computation time.

The Sweep Algorithm

```
forall the o ∈ Octants do
    forall the c ∈ Cells do
        ▷ c = (i, j, k)
        forall the d ∈ Directions[o] do
            ▷ d = (ν, μ, ξ)
            ε_x = 2ν/Δx;   ε_y = 2η/Δy;   ε_z = 2ξ/Δz;
            ψ[o][c][d] = (ε_x ψ_L + ε_y ψ_B + ε_z ψ_F + S) / (ε_x + ε_y + ε_z + Σ_t);
            ψ_R[o][c][d] = 2ψ[o][c][d] − ψ_L[o][c][d];
            ψ_T[o][c][d] = 2ψ[o][c][d] − ψ_B[o][c][d];
            ψ_BF[o][c][d] = 2ψ[o][c][d] − ψ_F[o][c][d];
            φ[k][j][i] = φ[k][j][i] + ψ[o][c][d] ∗ ω[d];
        end
    end
end
```

- 9 add or sub;
- 11 mul;
- 1 div (5 flops)
  $\rightarrow$ 25 flops per cell, per direction, per energy group.

The Spatial Sweep (*Diamond Differencing scheme*) (1/2)



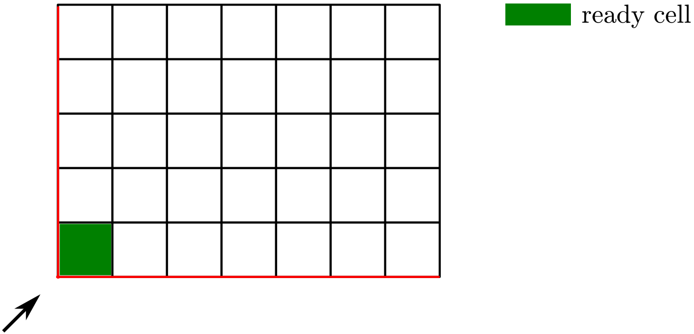
3D regular mesh with per cell, per angle, per energy group:

- 1 moment to update
- 3 incoming fluxes
- 3 outgoing fluxes

The Spatial Sweep (*Diamond Differencing scheme*) (2/2)

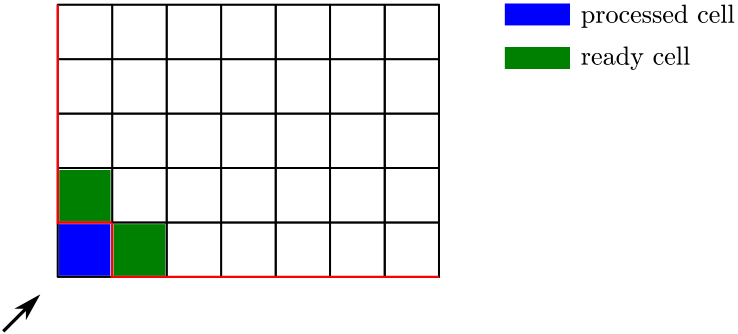
2D example of the spatial mesh for one octant

At the beginning, data are known only on the incoming faces



The Spatial Sweep (*Diamond Differencing scheme*) (2/2)

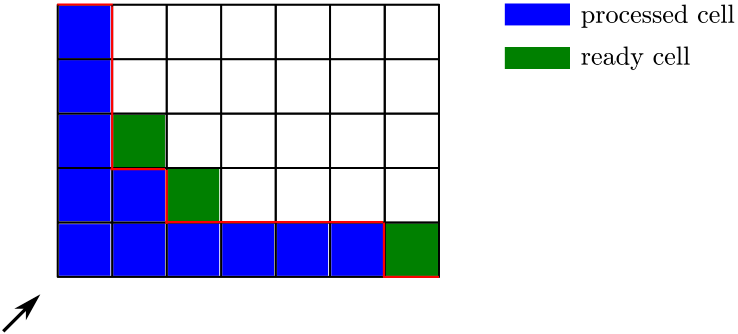
2D example of the spatial mesh for one octant



The Spatial Sweep (*Diamond Differencing scheme*) (2/2)

2D example of the spatial mesh for one octant

... after a few steps

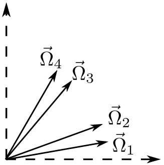


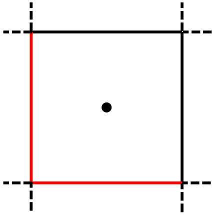
2
Parallelization Strategies

Many opportunities for parallelism

- Each level of discretization is a potentially independent computation:
  - energy group
  - angles
  - space
- All energy groups are computed together
- All angles are considered independent
  $\rightarrow$ This is not true when problems have boundary conditions
- All cell updates on a front are independent

Angular Parallelization Level (Very Low Level)



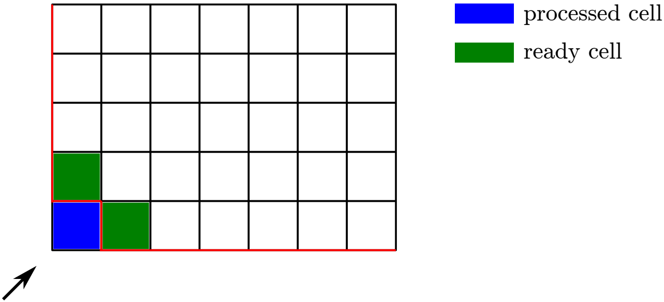


Several directions belong to the same octant:

- Vectorization of the computation
- Use of SIMD units at processor/core level
  $\rightarrow$ improve kernel performance

Spatial Parallelization

First level: granularity

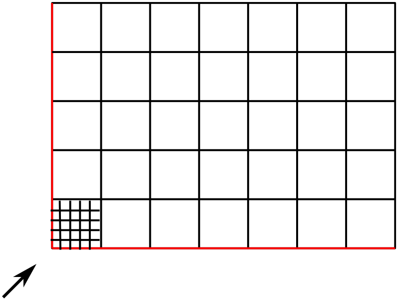


Grouping cells in MacroCells:

- Reduces thread scheduling overhead
- Similar to exploiting BLAS 3
- Reduces overall parallelism

Spatial Parallelization

First level: granularity



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- Similar to exploiting BLAS 3
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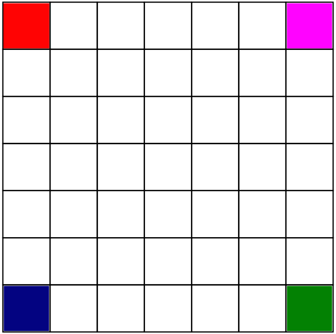
Octant Parallelization

Case of Vacuum Boundary Conditions

When using vacuum boundary conditions, all octants are independent from each other



Octant Parallelization

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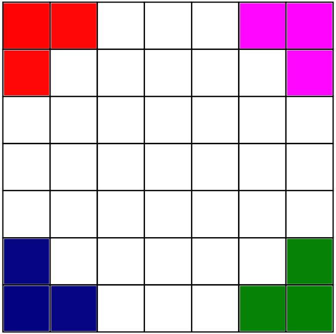

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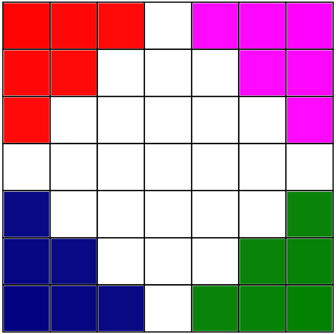
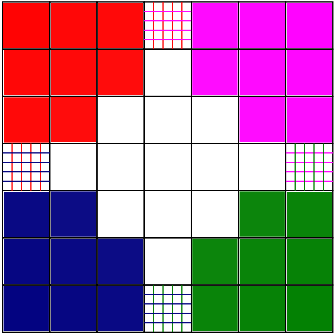


Octant Parallelization

Case of Vacuum Boundary Conditions

Concurrent access to a cell (or MacroCell) are protected by mutexes.



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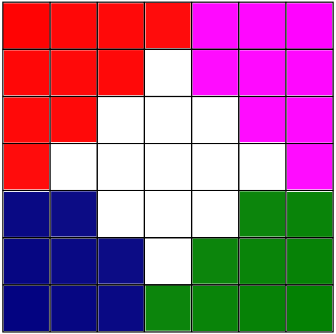
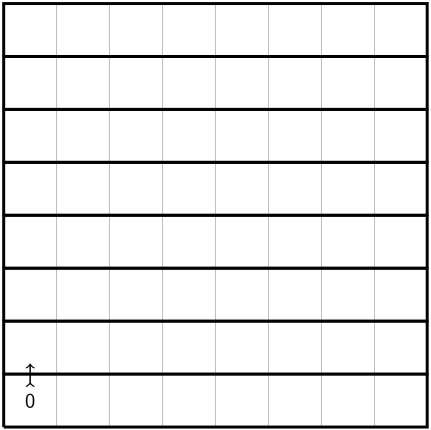
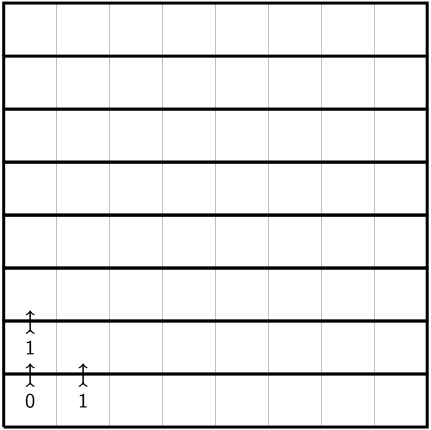


3
Sweep Theoritical Model

Basic ideas - Flat Model



Basic ideas - Flat Model



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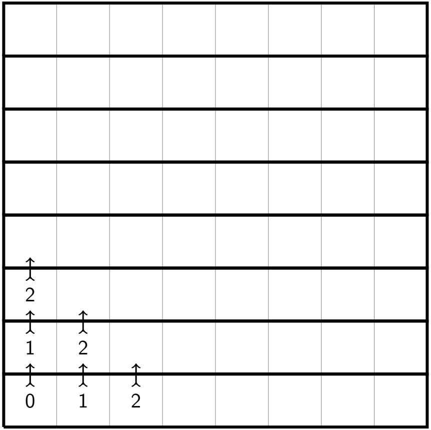
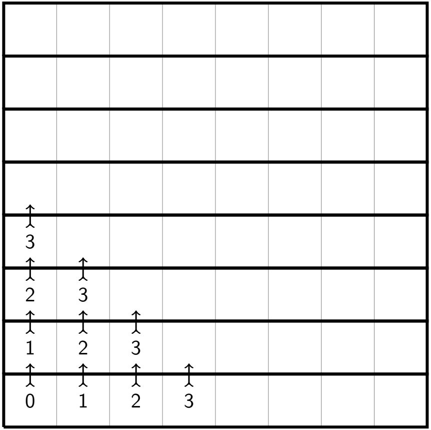


Basic ideas - Flat Model



- 1D block distribution
- Requires:
  - 14 tasks
  - 7 communications

Basic ideas - Flat Model

7	8	9	10	11	12	13	14
6	7	8	9	10	11	12	13
5	6	7	8	9	10	11	12
4	5	6	7	8	9	10	11
3	4	5	6	7	8	9	10
2	3	4	5	6	7	8	9
1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7

- 1D block distribution
- Requires:
  - 14 tasks
  - 7 communications

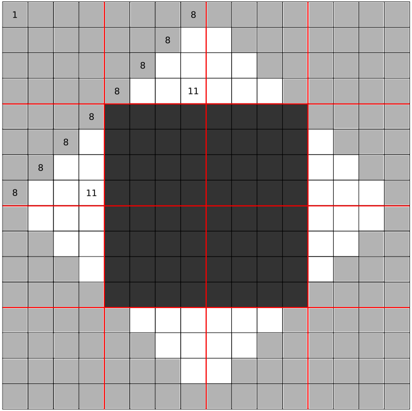
Formulas (Adams et al.)

We define the efficiency of the sweep algorithm as follow:

$$\begin{aligned}\epsilon &= \frac{T_{task} N_{tasks}}{(N_{tasks} + N_{idle}) * (T_{task} + T_{comm})} \\ &= \frac{1}{(1 + N_{idle}/N_{tasks}) * (1 + T_{comm}/T_{task})}\end{aligned}$$

Objective: **Minimize** N_{idle}

Filling the pipeline



For 3D block distribution

The minimal number of idle steps are those required to reach the cube center:

$$N_{idle}^{min} = P_x + \delta_x - 2 + P_y + \delta_y - 2 + P_z + \delta_z - 2$$

where $\delta_u = 0$, if P_u is even, 1 otherwise.

Objective: **Minimize the sum** $P + Q + R$, where $P \times Q \times R$ is the process grid.
$\rightarrow$ Hybrid MPI-Thread implementation should allow this

Hybrid MPI-Thread model

7	8	9	10	11	12	13	14
6	7	8	9	10	11	12	13
5	6	7	8	9	10	11	12
4	5	6	7	8	9	10	11
3	4	5	6	7	8	9	10
2	3	4	5	6	7	8	9
1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7

- Requires:
  - 14 tasks
  - 2 communications instead of 7

Hybrid MPI-Thread model

7	8	9	10	11	12	13	14
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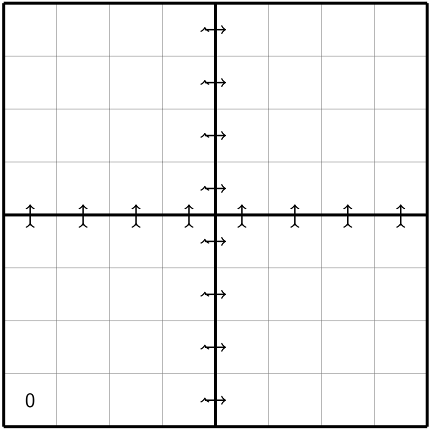
1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7

- Requires:
  - 14 tasks
  - 2 communications instead of 7
- Only 2 cores per node!!!

Hybrid MPI-Thread model

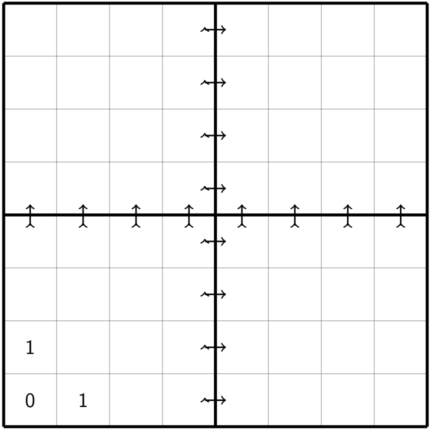
Scheduling by front



- Natural order: follow the fronts
- Requires 19 steps

Hybrid MPI-Thread model

Scheduling by front



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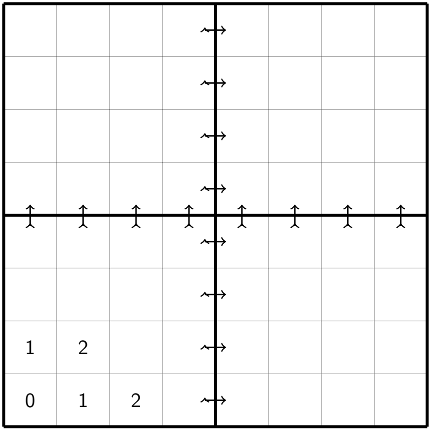

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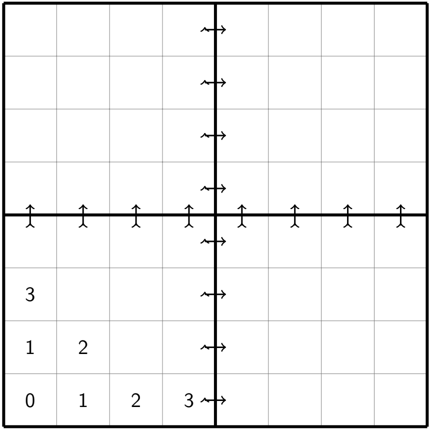

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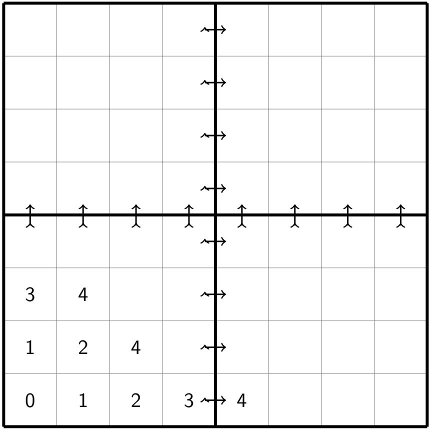

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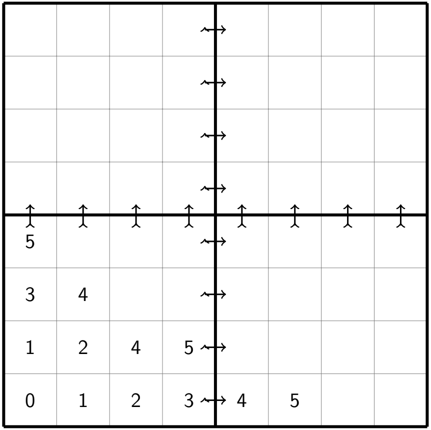

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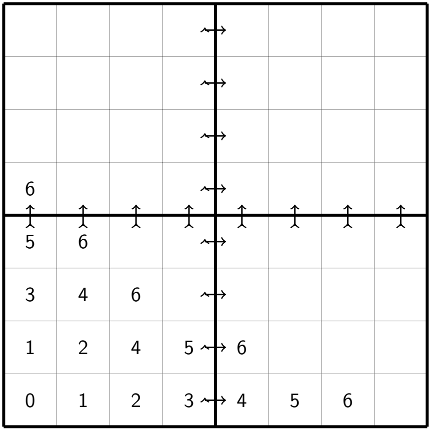

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Hybrid MPI-Thread model

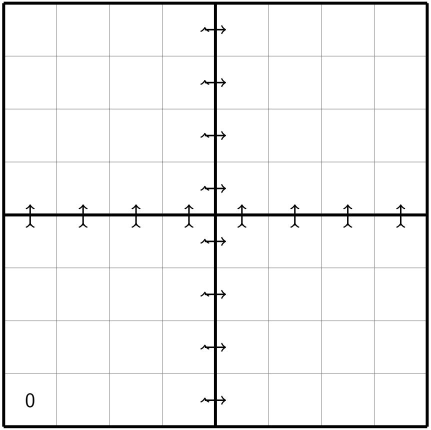
Scheduling by front

11	12	13	14	16	17	18	19
9	10	12	13	14	15	17	18
7	8	10	11	12	13	15	16
6	7	8	9	11	12	13	14
5	6	7	8	10	11	12	13
3	4	6	7	8	9	11	12
1	2	4	5	6	7	9	10
0	1	2	3	4	5	6	8

- Natural order: follow the fronts
- Requires 19 steps

Hybrid MPI-Thread model

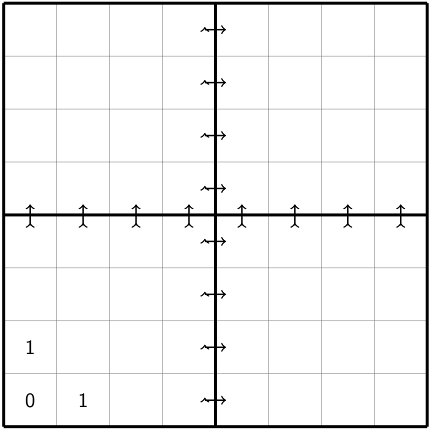
Favour one direction



- Give priority to one direction of the octant
- Might delay other directions
- Requires **18** steps

Hybrid MPI-Thread model

Favour one direction



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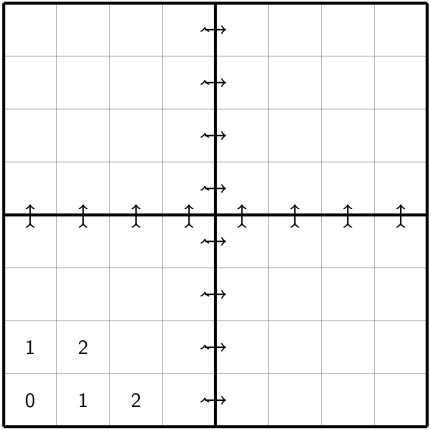

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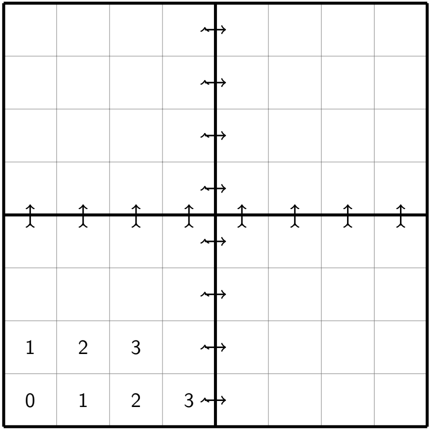

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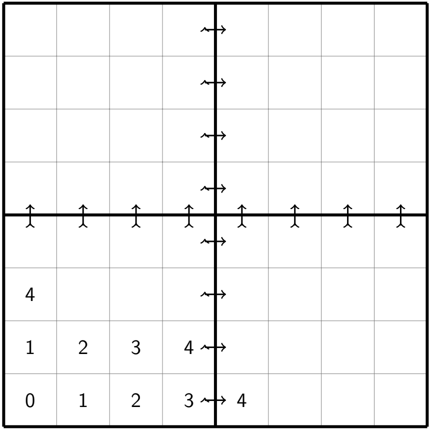

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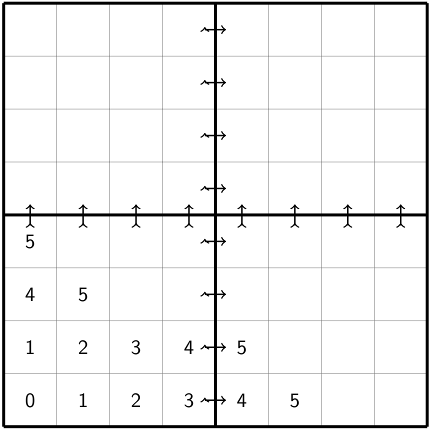

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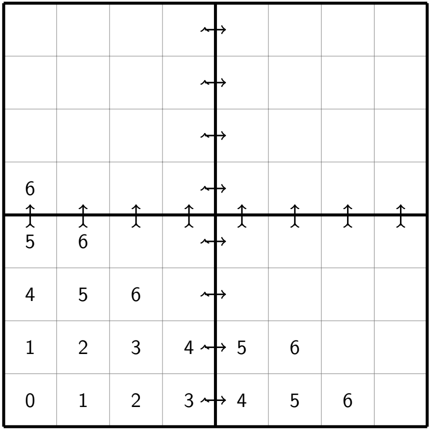

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Hybrid MPI-Thread model

Favour one direction

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Hybrid MPI-Thread model

Priority used

For 3D distribution grid $P \times Q \times R$ with $P > Q > R$, we favour the largest direction first.

4
DOMINO on top of PaRSEC

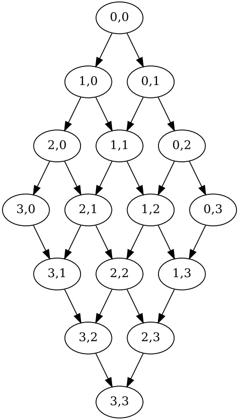
DOMINO on top of PaRSEC

Implementation

- Only one kind of task:
  - Associated to one MacroCell
  - All energy group
  - All directions included in one octant
    $\rightarrow$ 8 tasks per MacroCell
  - No dependencies from one octant to another
    $\rightarrow$ protected by mutexes
- Simple algorithm to write in JDF
- Require a data distribution:
  - Independent from the algorithm: 2D, 3D, cyclic or not, ...
  - For now: Block-3D (Non cyclic) with a $P \times Q \times R$ grid
- Fluxes on faces are dynamically allocated/freed by the runtime

DOMINO JDF Representation (1 sweep in 2D)

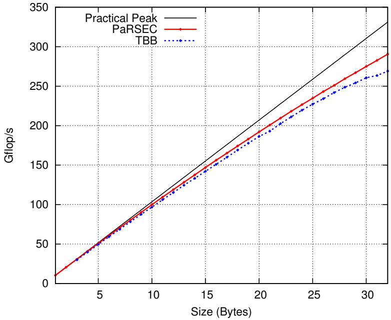
```
T(a, b)
// Execution space
a = 0 .. 3
b = 0 .. 3

// Parallel partitioning
: mcg(a, b)

// Parameters
RW X   <- (a != 0) ? X  T(a-1, b)
       -> (a != 3) ? X  T(a+1, b)

RW Y   <- (b != 0) ? Y  T(b, b-1)
       -> (b != 3) ? Y  T(b, b+1)

RW MCG <- mcg(a, b)
       -> mcg(a, b)

BODY
{
  computePhi ( MCG, X, Y, ... );
}
END
```



5
Results

Shared Memory Results (PaRSEC VS Intel TBB)

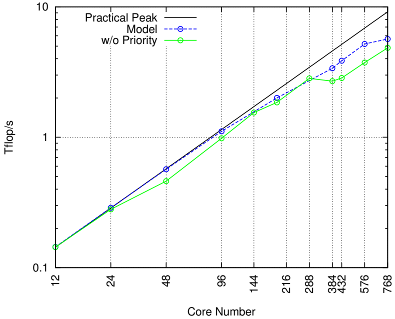
32 cores – Intel X7560



- Mesh size: $480 \times 480 \times 480$; *Level Symmetric* S16 (288 directions)
- Achieves 291 Gflop/s (51% of Theoretical Peak Perf.)

Distributed Memory Results – Hybrid

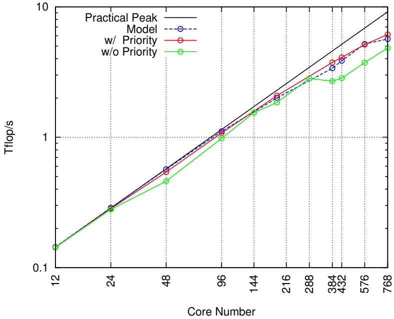
IVANOE – 768 cores (64 nodes of 12 cores) – Intel X7560



- Mesh size: $480 \times 480 \times 480$; *Level Symmetric* S16 (288 directions)
- Parallel efficiency: 52.7%
- 4.8 Tflop/s (26.8% of Theoretical Peak Perf.) at 768 cores

Distributed Memory Results – Hybrid

IVANOE – 768 cores (64 nodes of 12 cores) – Intel X7560

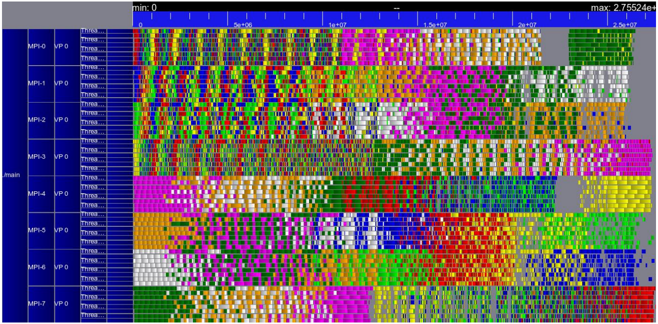


- Mesh size: $480 \times 480 \times 480$; *Level Symmetric* S16 (288 directions)
- Parallel efficiency: 66.8%
- 6.2 Tflop/s (34.4% of Theoretical Peak Perf.) at 768 cores

Distributed Memory Results – Hybrid

Execution traces

Execution trace for a run on 8 nodes (2, 2, 2) (w/o priorities).



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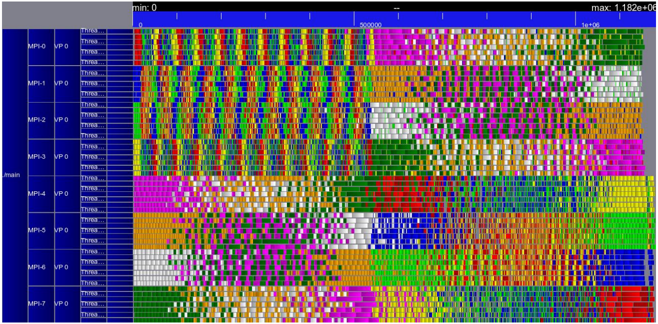
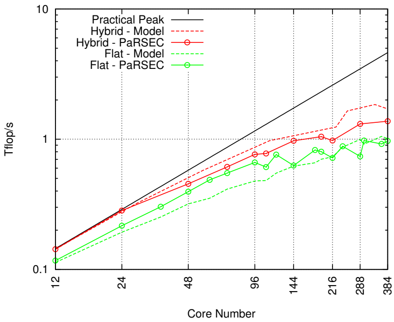


Distributed Memory Results – Flat vs Hybrid

IVANOE – 384 cores – Intel X7560



- Mesh size: $120 \times 120 \times 120$; *Level Symmetric* S16 (288 directions)
- Flat model: Overlap is not integrated into the model

6 Conclusion and future works

Conclusion and Future Work

Conclusion

- Efficient implementation on top of PaRSEC
  - Less than 2 weeks to be implemented
  - Comparable to Intel TBB in shared memory
- *Simple* multi-level implementation:
  - Code vectorization (angular direction)
  - Block algorithm (MacroCells)
  - Hybrid MPI-Thread implementation

Future work

- Fix the hybrid model to try new scheduling and get the best data distribution out of it
- Experiments on Intel Xeon Phi
- Model of the symmetric case

Thanks !