Flexible Fast Multipole Method for Magnetic Simulations

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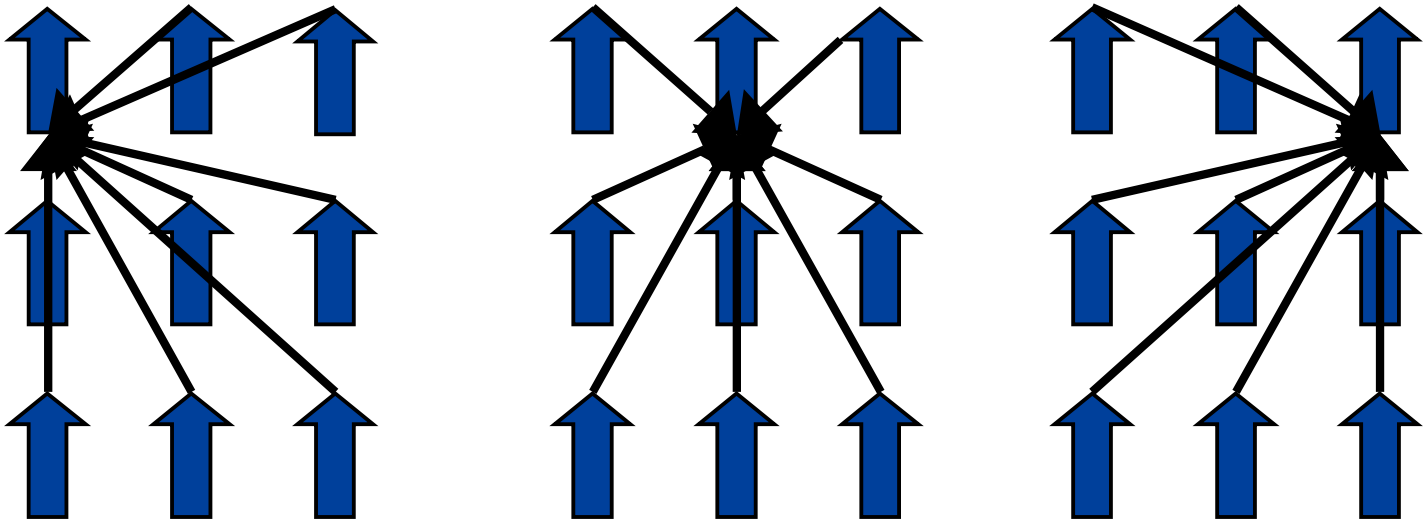
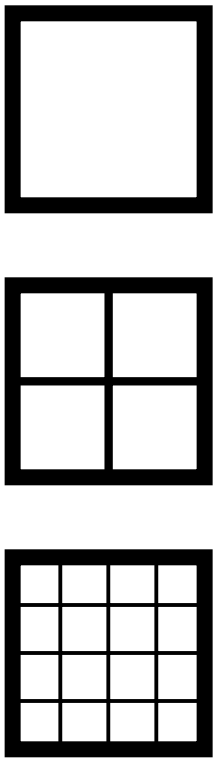
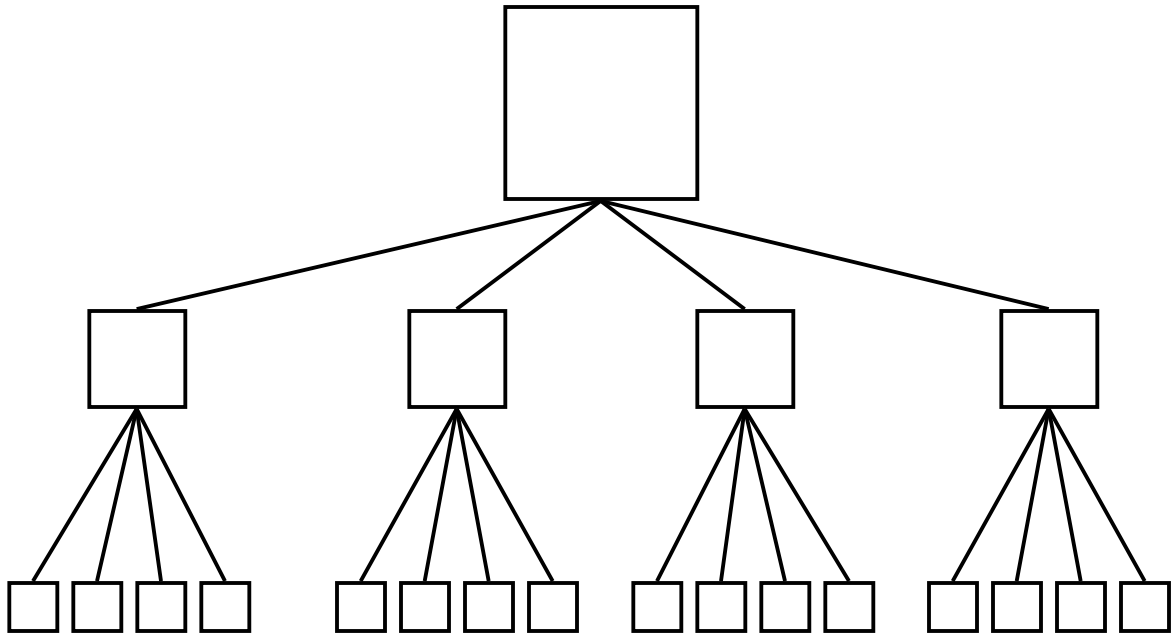
Dipole-dipole interactions



- **Direct: O(** N^2 **)**
- **FFT: O(** $N \ln N$ **)**
- **FMM: O(** N **)**

Fast Multipole Method





Each box has
one expansion for sources,
one for local field

Concept: expansion of 3d function

Solid Harmonic

$$\phi(r,\theta,\varphi) = \sum_{i=0}^{p} \sum_{j=-i}^{i} M_{i,j} r^{-(i+1)} Y_{i,j}(\theta,\varphi)$$

$$\psi(r,\theta,\varphi) = \sum_{i=0}^{p} \sum_{j=-i}^{i} M_{i,j} r^{i} Y_{i,j}(\theta,\varphi)$$

implemented at
Oak Ridge

Cartesian

$$\phi(x,y,z) = \sum_{i=0}^{p} \sum_{j=0}^{p-i} \sum_{k=0}^{p-i-j} \frac{M_{i,j,k}}{i!\,j!\,k!} \frac{x^i y^j z^k}{r^{2(i+j+k)+1}}$$

$$\psi(x,y,z) = \sum_{i=0}^{p} \sum_{j=0}^{p-i} \sum_{k=0}^{p-i-j} \frac{M_{i,j,k}}{i!\,j!\,k!} x^i y^j z^k$$

implemented at
Univ. of Alabama

Ψ-*Mag* implementation of Fast Multipole can use these interchangably

Ψ-*Mag* uses Generic Programming

The set of requirements associated with a certain type of thing is called a concept.

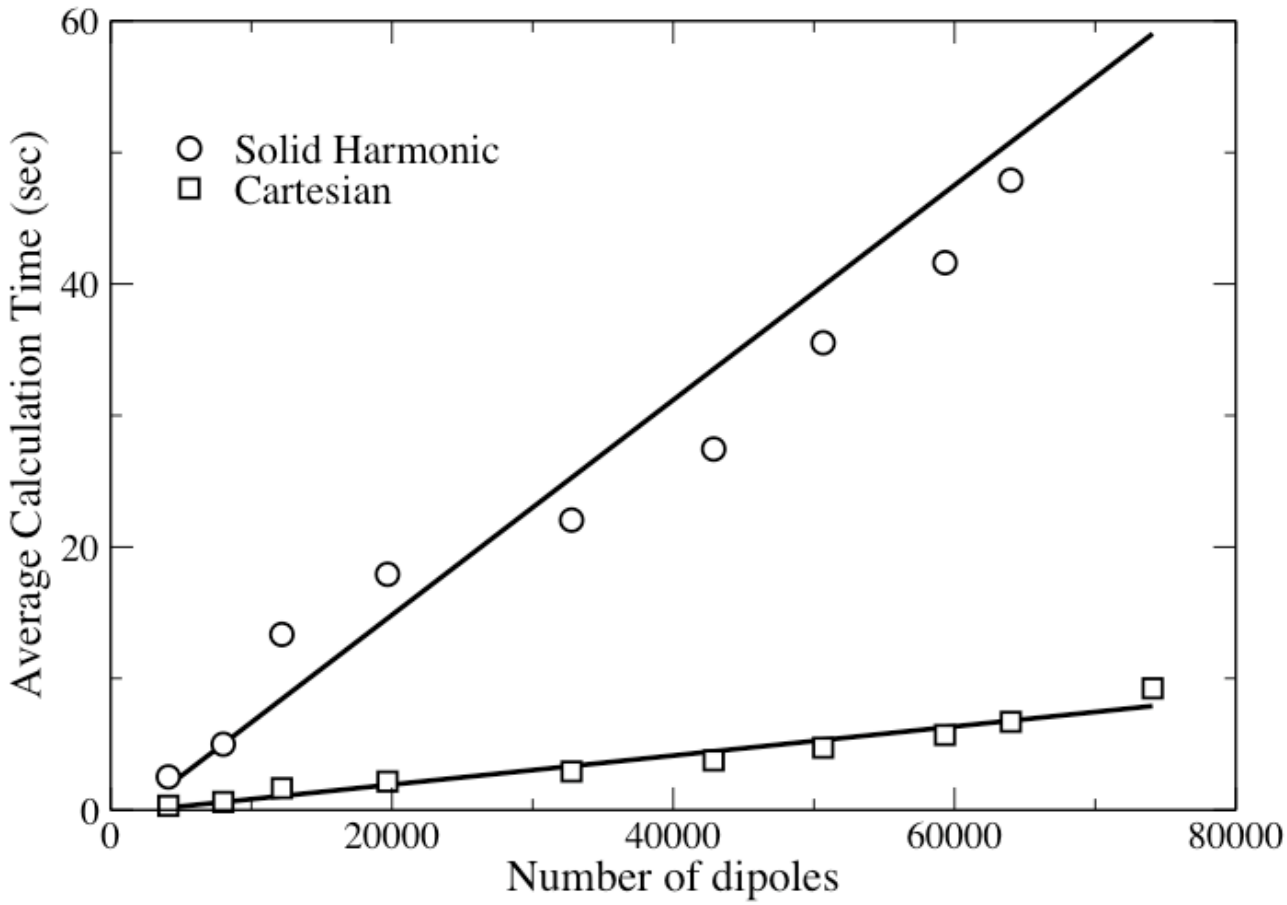
The classes which implement those requirements are called models.

Can code once details like breaking up space.
Can provide new expansions as needed.

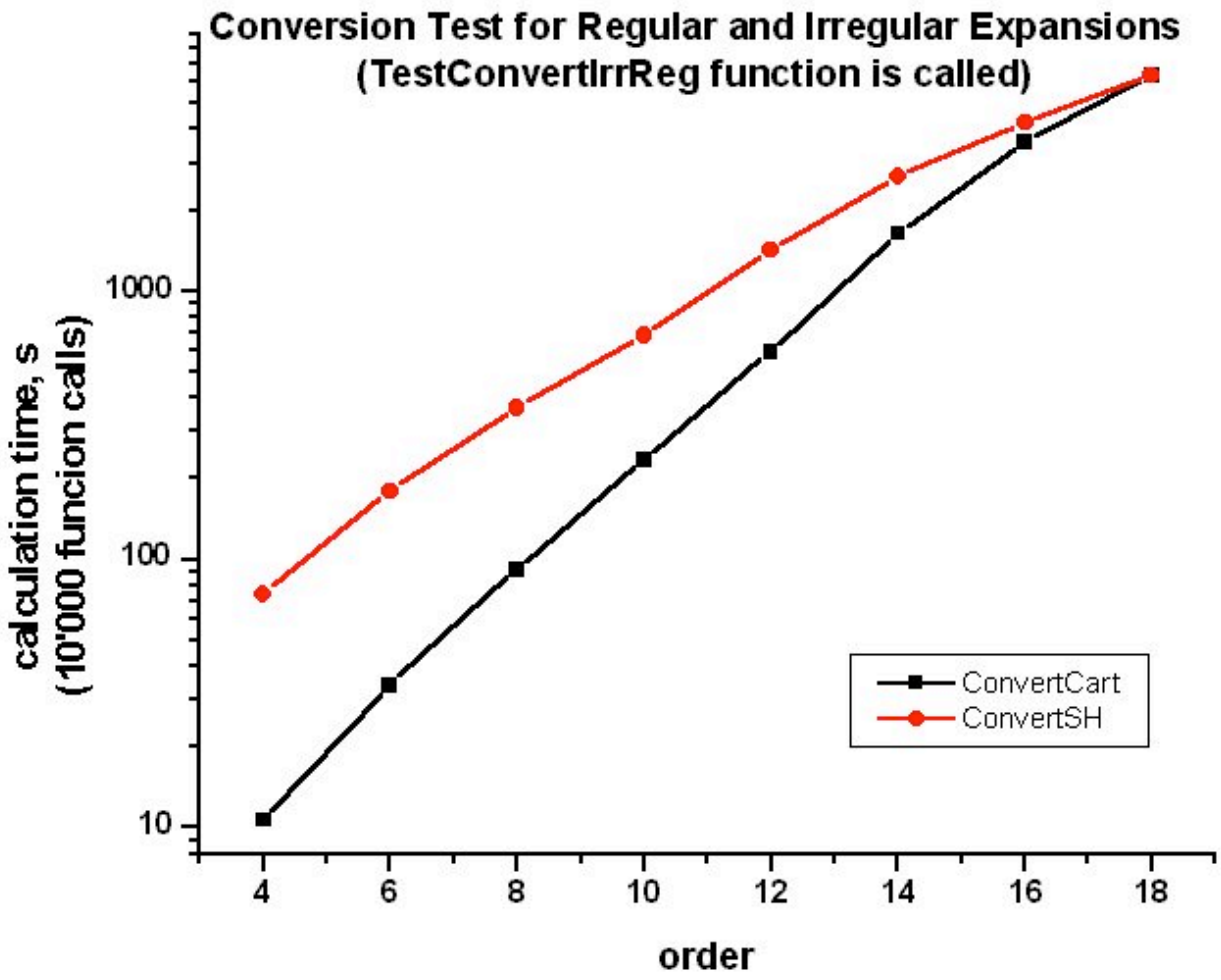
Test Calculation

- Randomly oriented dipoles
- Cubic Lattice
- 4 processors of IBM RS/6000
- p=4

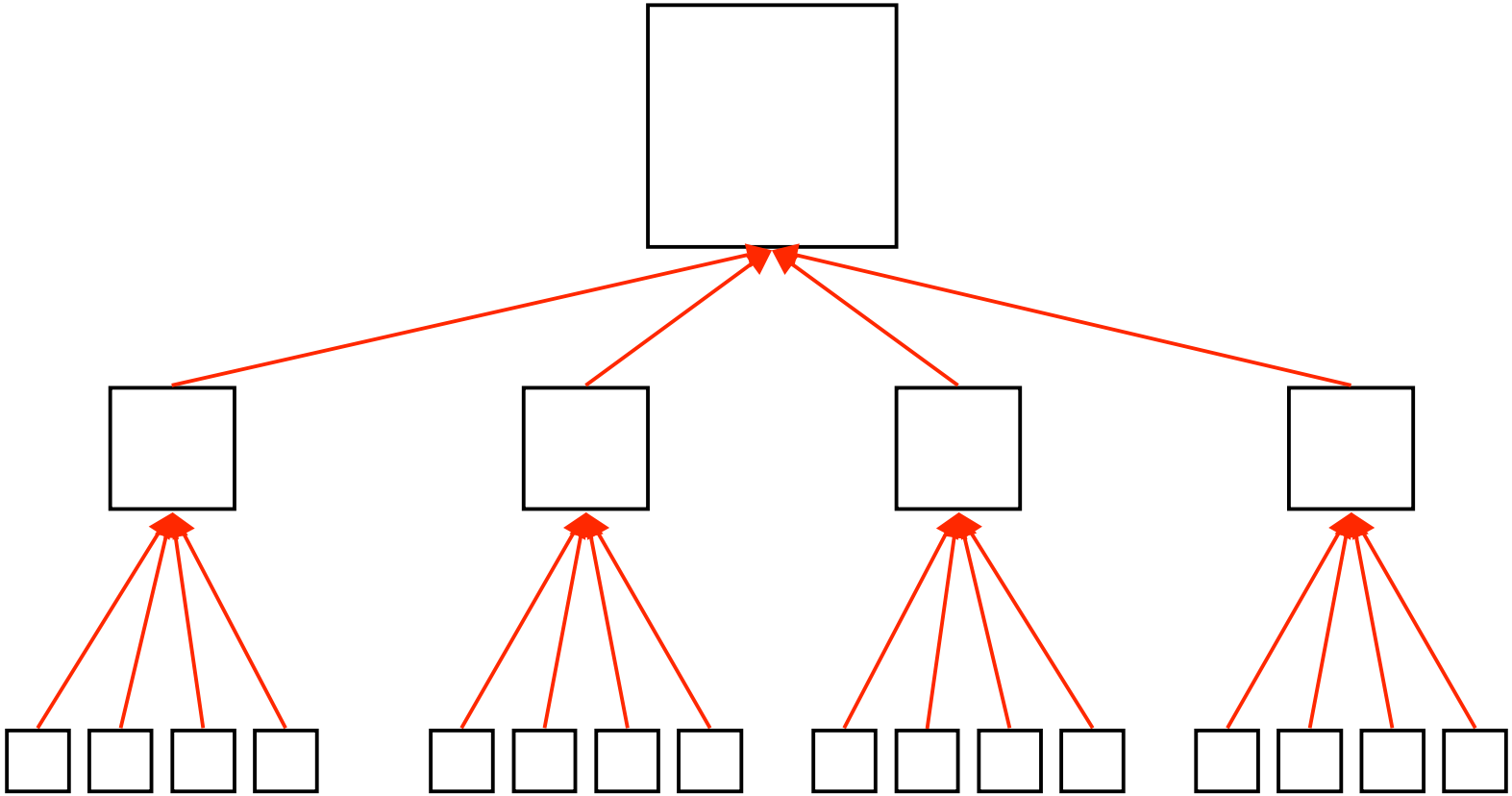
Calculation time



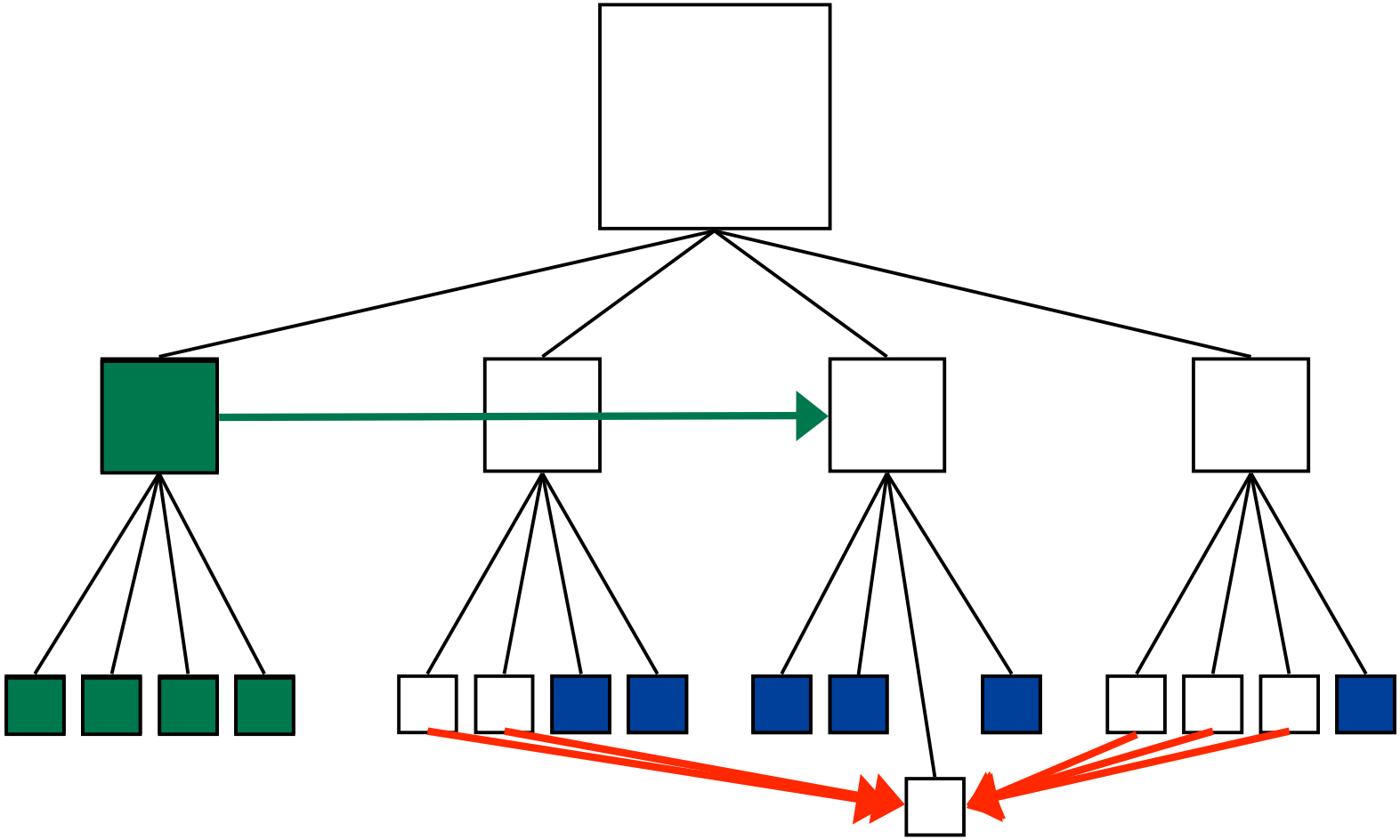
Cartesian not always optimal



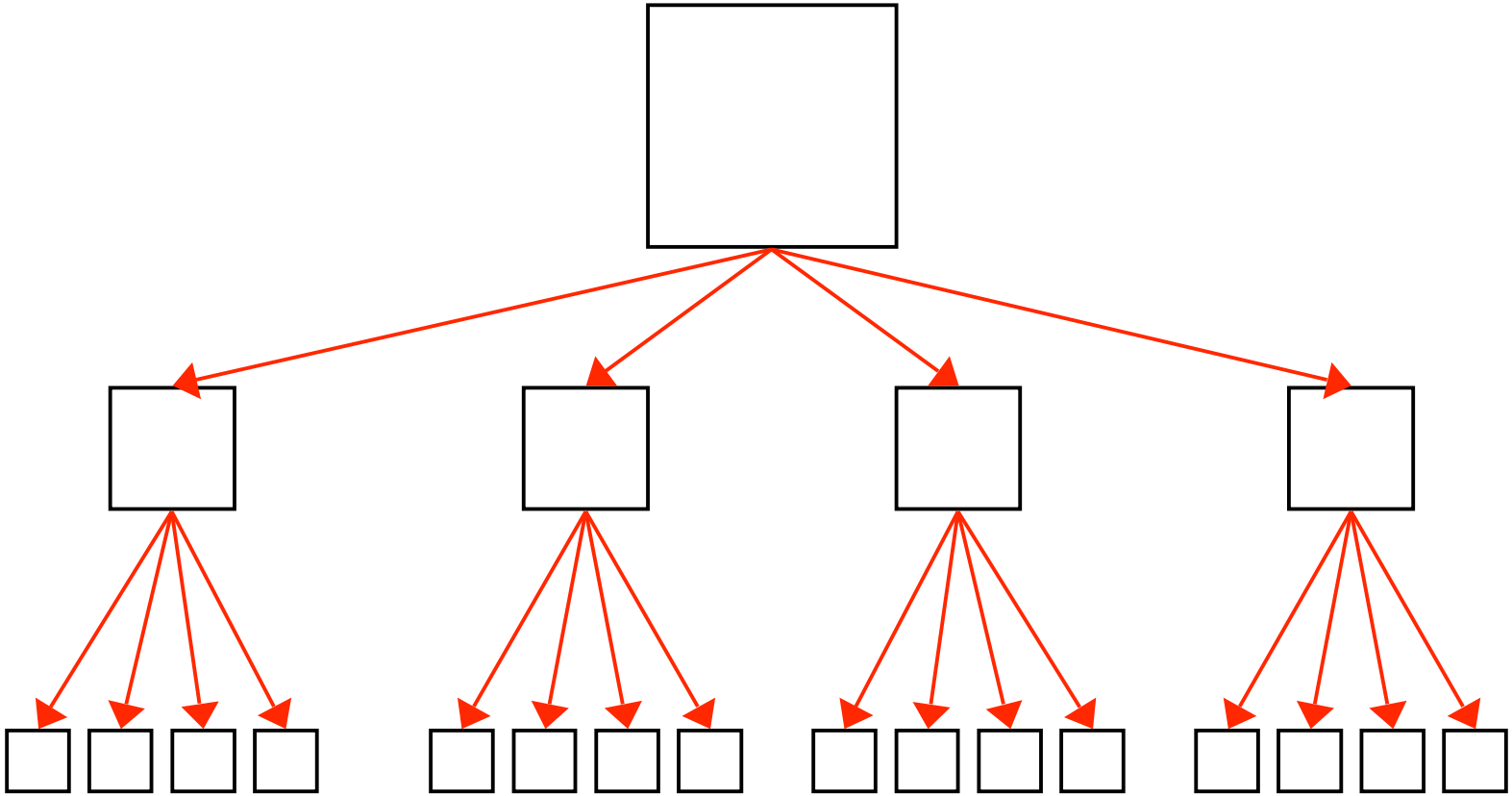
Build-up Multipole Expansions



Potential due to far-away sources



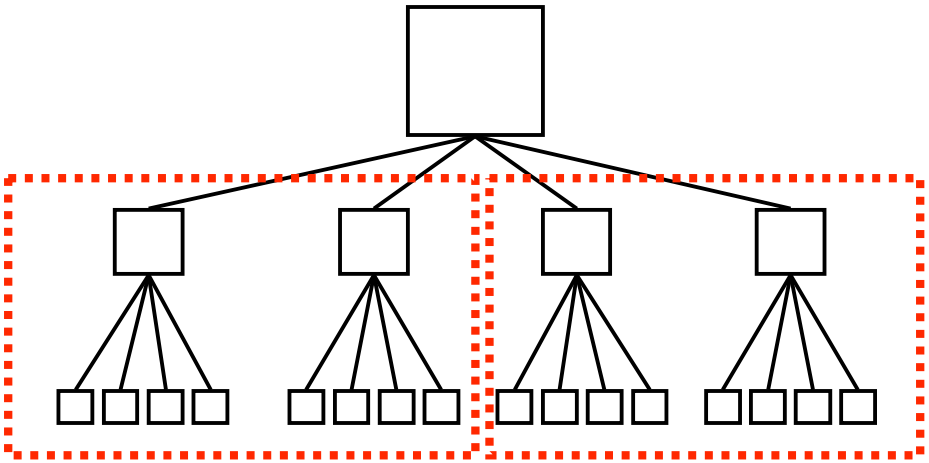
Contributions from the really far



Scaling on multiple processors

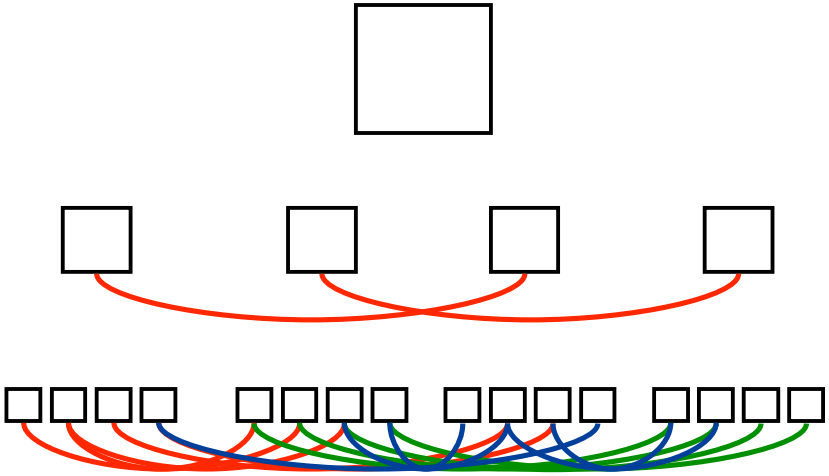
space decomposition

- local communication
- more communications
- problem dependent

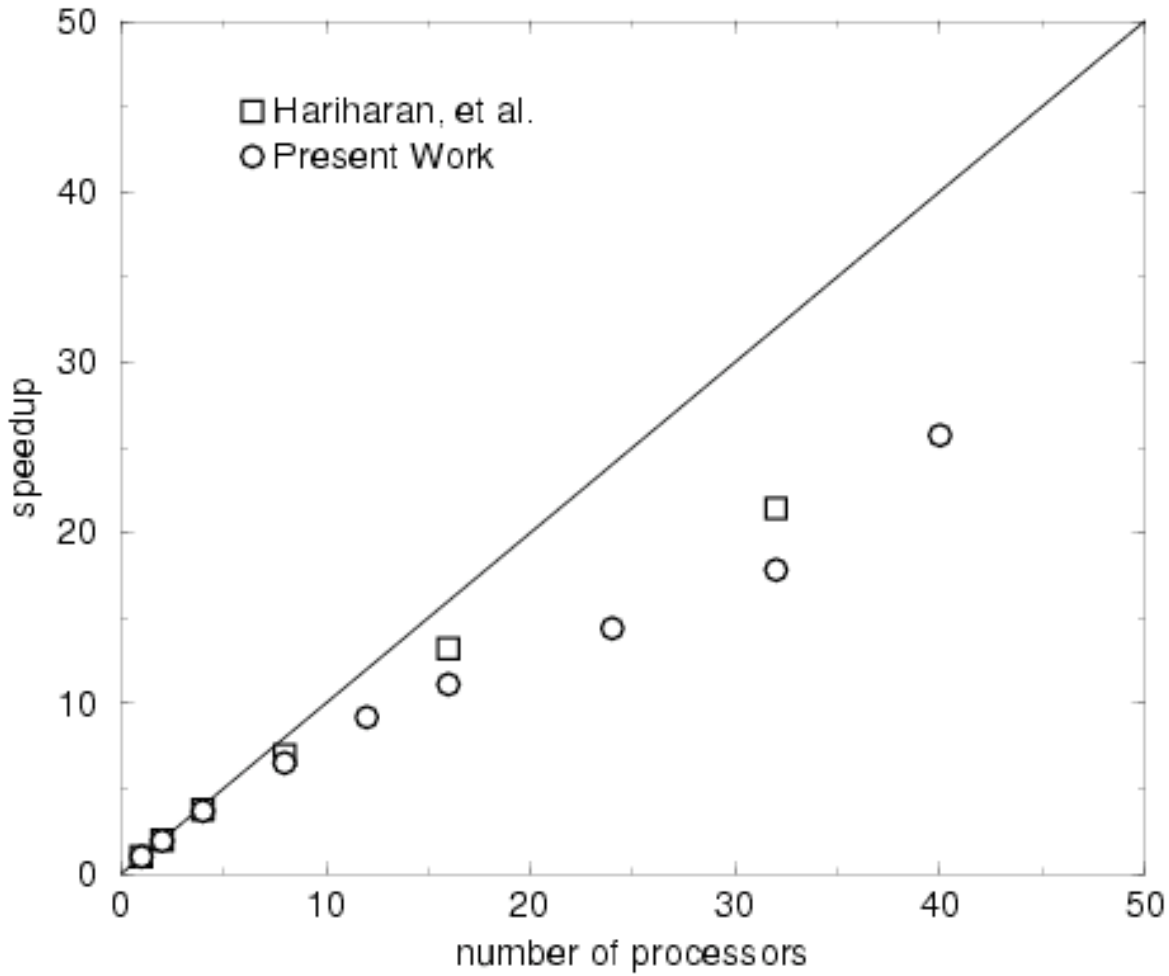


task decomposition

- all-to-all communication
- once communication per calculation
- problem independent



Multiple-processor speedup



Summary

- Generic/Flexible Fast Multipole
- O(N) computational effort
- Scales well on up to 32 processors
- Direct comparison of two expansions
- Could be used to compare different methods
- Acknowledgements

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