Fast Computing of Boundary Integral Equation Method by a Special-purpose Computer

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1. Introduction

Overcoming the cost problem in
Boundary Integral Equation Method (BIEM)

↓ breakthrough

Fast algorithms (B&H, FMM, ...)

applications : Laplace, Helmholtz, electromagnetism, elastostatics, elastodynamics, ...

↓ further acceleration !!

Special-purpose computer (MDGRAPE-2)

- conventional (direct sum.) BIEM
- fast BIEM (future work)

● Outline

1. Introduction

2. Overview of BIEM

3. Overview of MDGRAPE-2

4. Application of MDGRAPE-2 to conventional BIEM

5. Application of MDGRAPE-2 to fast BIEM

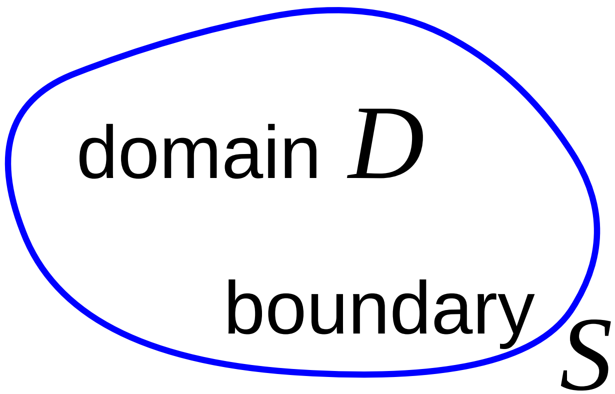
6. Conclusion

2. Overview of BIEM

● Formulation of BIEM

- Boundary value problem of PDE

  ↓ Green's function G

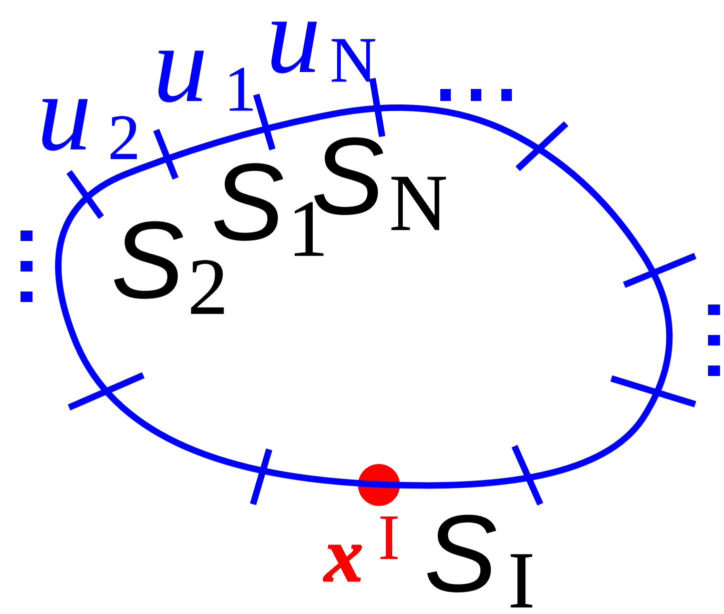


- Boundary Integral Equation (BIE) :

$$\underbrace{\int_S G(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y}) dS_y}_{\text{layer potential}} = b(\boldsymbol{x})$$

- Discretisation
  - piecewise constant element
  - collocation method

$$\underbrace{\sum_{J=1}^{N} u_J \int_{S_J} G(\boldsymbol{x}^I, \boldsymbol{y})\, dS_y}_{\text{layer potential}} = b(\boldsymbol{x}^I)$$

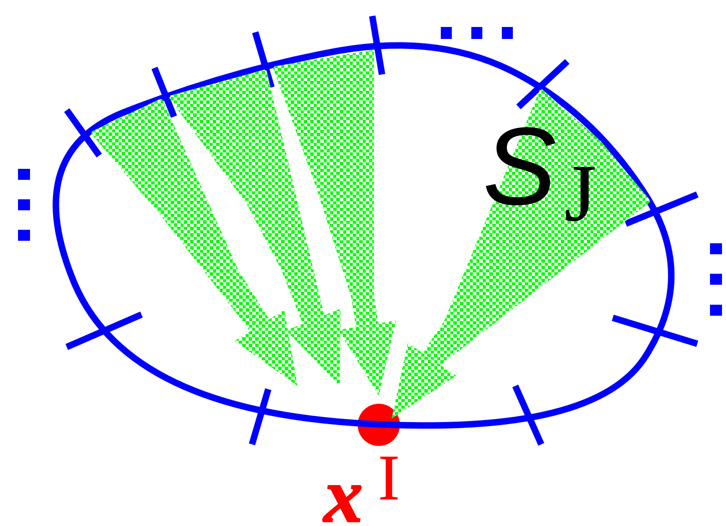


- Solve iteratively

  evaluation of layer potential

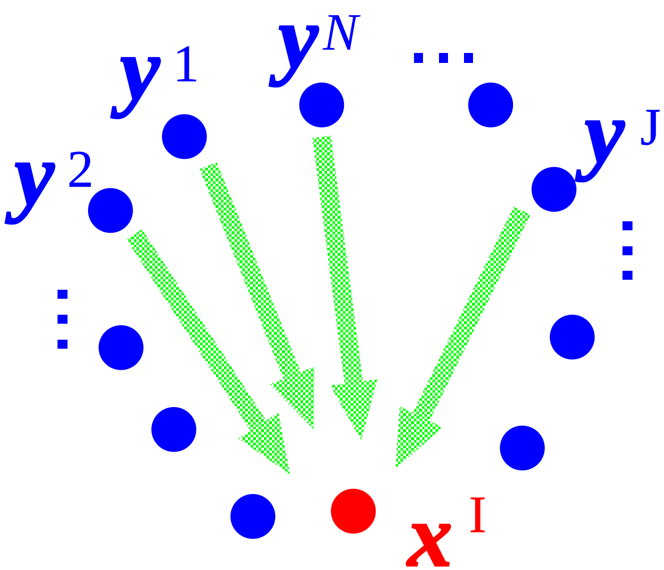
  $\downarrow$

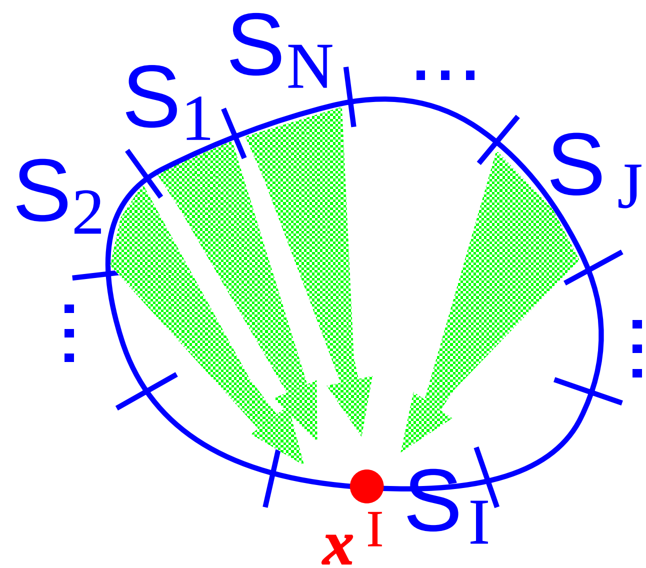
  cost is $O(N^2)$!!



• Similarity to N-body simulation

N-body		BIEM
pairwise interaction	$\leftrightarrow$	layer potential





$\downarrow$

special-purpose computer $\longrightarrow$ hopeful

GRAPE, MDGRAPE-2...

3. Overview of MDGRAPE-2

● System

General–purpose Computer	$\dashrightarrow$ $\dashleftarrow$	MDGRAPE-2
host (master)		slave
light works $O(N)$		heavy work $O(N^2)$
		||
		pairwise interaction
		100–1000 times faster

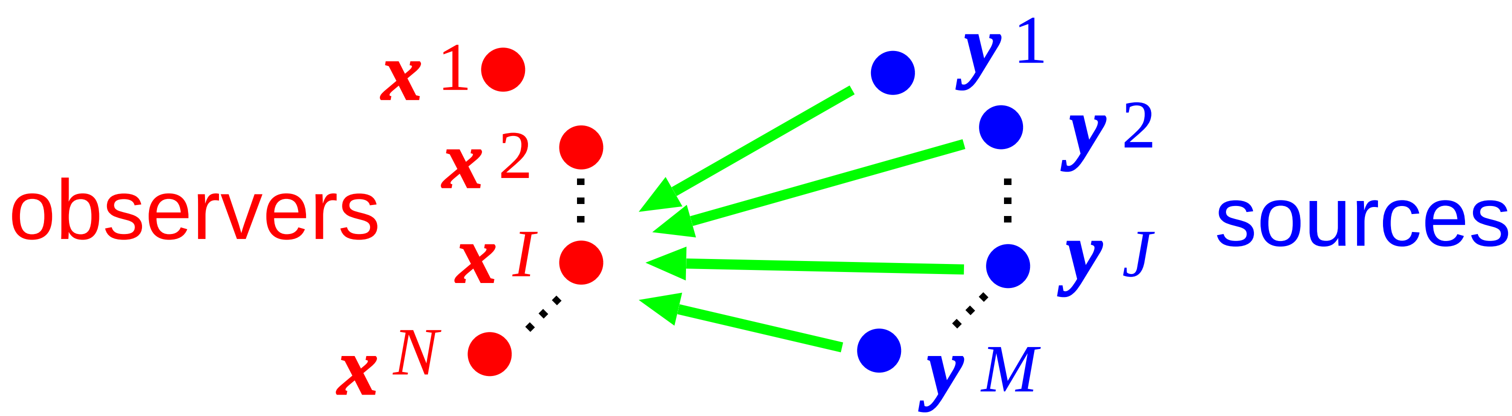
● Function of MDGRAPE-2

compute pairwise interactions among particles :

$$\text{“potential”} \quad : \quad \phi_I = \sum_{J=1}^{M} b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|)$$

$$\text{“force”} \quad : \quad \boldsymbol{f}^I = \sum_{J=1}^{M} b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|)(\boldsymbol{x}^I - \boldsymbol{y}^J)$$

$$\text{for } I = 1, 2, \ldots, N$$



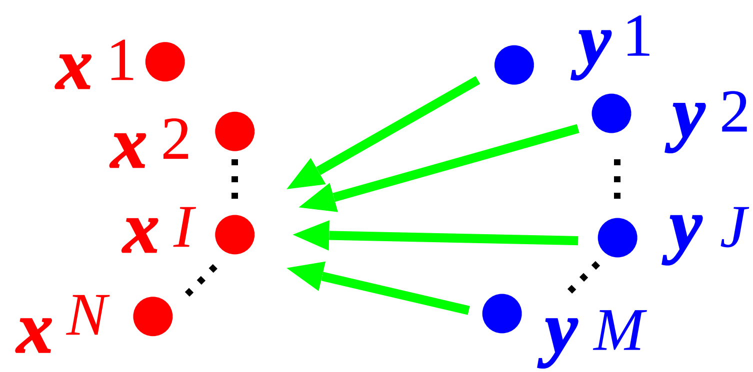
• What's MDGRAPE-2

MDGRAPE-2 is a vector-parallel computer

do $I = 1,\ N$

do $J = 1,\ M$

$$\phi_I = \phi_I + b_J\, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|)$$

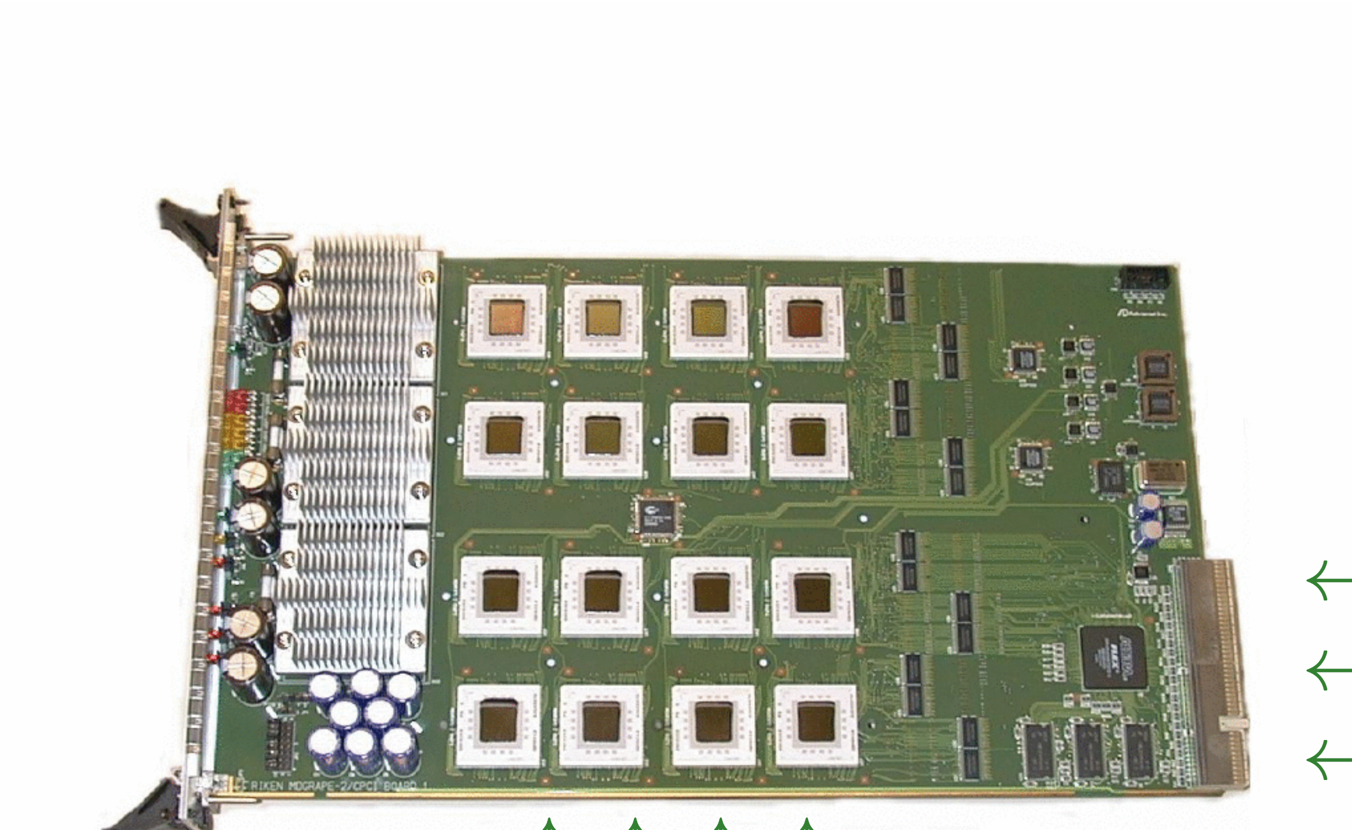


$\Downarrow$

vectorisation w.r.t. J and parallelisation w.r.t I
(hardwired pipeline) (use pipelines parallely)

$\longrightarrow$ 10^8 pairs/second/pipeline

● MDGRAPE-2 board



← ← I/O ← interface

↑ ↑ ↑ ↑ custom chips

CompactPCI version (128 pipelines; 100MHz) developed by RIKEN

4. Application of MDGRAPE-2 to conventional BIEM

KEY POINT

Describe a layer potential

$$\int_S G(\boldsymbol{x}^I, \boldsymbol{y}) u(\boldsymbol{y}) dS_y$$

in the form of

$$\begin{aligned} \phi_I &= \sum_{J=1}^{M} b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|), \\ \boldsymbol{f}^I &= \sum_{J=1}^{M} b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|)(\boldsymbol{x}^I - \boldsymbol{y}^J) \end{aligned}$$

• Laplace equation in 3D

Laplace eq. :

$$\Delta u(\boldsymbol{x}) = 0 \quad \text{in } D \subset \mathbb{R}^3$$

Boundary Integral Equation :

$$\frac{1}{2}u(\boldsymbol{x}) = \int_S \left(G(\boldsymbol{x}-\boldsymbol{y})q(\boldsymbol{y}) - \frac{\partial G(\boldsymbol{x},\boldsymbol{y})}{\partial n_y}u(\boldsymbol{y}) \right) dS_y \quad \text{for } \boldsymbol{x} \in S$$

Fundamental solution:

$$G(\boldsymbol{x}-\boldsymbol{y}) = \frac{1}{4\pi\left|\boldsymbol{x}-\boldsymbol{y}\right|}$$

• Evaluation of the single layer potential

$$\int_S G(\boldsymbol{x}^I - \boldsymbol{y})q(\boldsymbol{y})dS_y$$

$$\simeq \sum_{j=1}^{N} q_j \int_{S_j} \frac{1}{4\pi|\boldsymbol{x}^I - \boldsymbol{y}|}dS_y$$

$$\simeq \sum_{j=1}^{N} q_j \sum_{k=1}^{M} \frac{w_k \Delta_j}{4\pi|\boldsymbol{x}^I - \boldsymbol{y}^{j,k}|}$$

(w_k : weight, Δ_j : area)

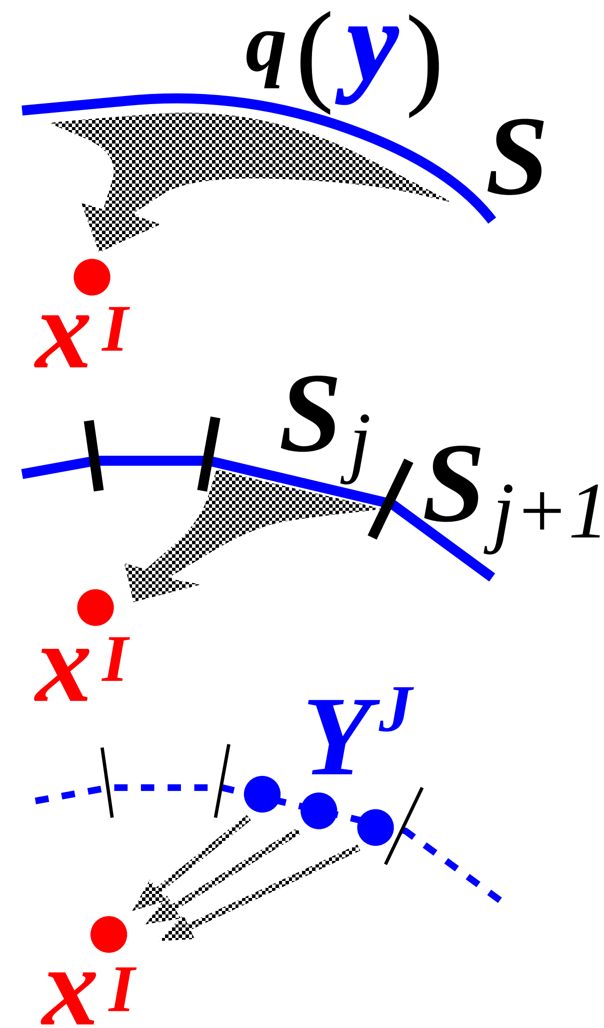
$$= \sum_{J=1}^{NM} \frac{Q_J}{|\boldsymbol{x}^I - \boldsymbol{Y}^J|}$$

$$\Updownarrow$$

$$\phi_I = \sum_J b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|), \quad g(x) \equiv 1/x$$

$$\downarrow$$

Drive MDGRAPE-2 once in potential-mode



• Evaluation of the double layer potential

$$\int_S \frac{\partial G(\boldsymbol{x}^I - \boldsymbol{y})}{\partial n_y} u(\boldsymbol{y}) dS_y$$

$$= \sum_J \frac{U_1^J(x_1^I - Y_1^J)}{\left|\boldsymbol{x}^I - \mathbf{Y}^J\right|^3} + \sum_J \frac{U_2^J(x_2^I - Y_2^J)}{\left|\boldsymbol{x}^I - \mathbf{Y}^J\right|^3} + \sum_J \frac{U_3^J(x_3^I - Y_3^J)}{\left|\boldsymbol{x}^I - \mathbf{Y}^J\right|^3}$$

$$\Updownarrow$$

$$\boldsymbol{f}^I = \sum_{J=1}^{M} b_J \, g(|\boldsymbol{x}^I - \boldsymbol{y}^J|)(\boldsymbol{x}^I - \boldsymbol{y}^J), \quad g(x) \equiv 1/x^3$$

$$\downarrow$$

Drive MDGRAPE-2 three times in “force” mode

• Application to other BIEMs

- Helmholtz equation in 2, 3D
- electromagnetism (EFIE & MFIE) in 3D
- elastostatics in 3D

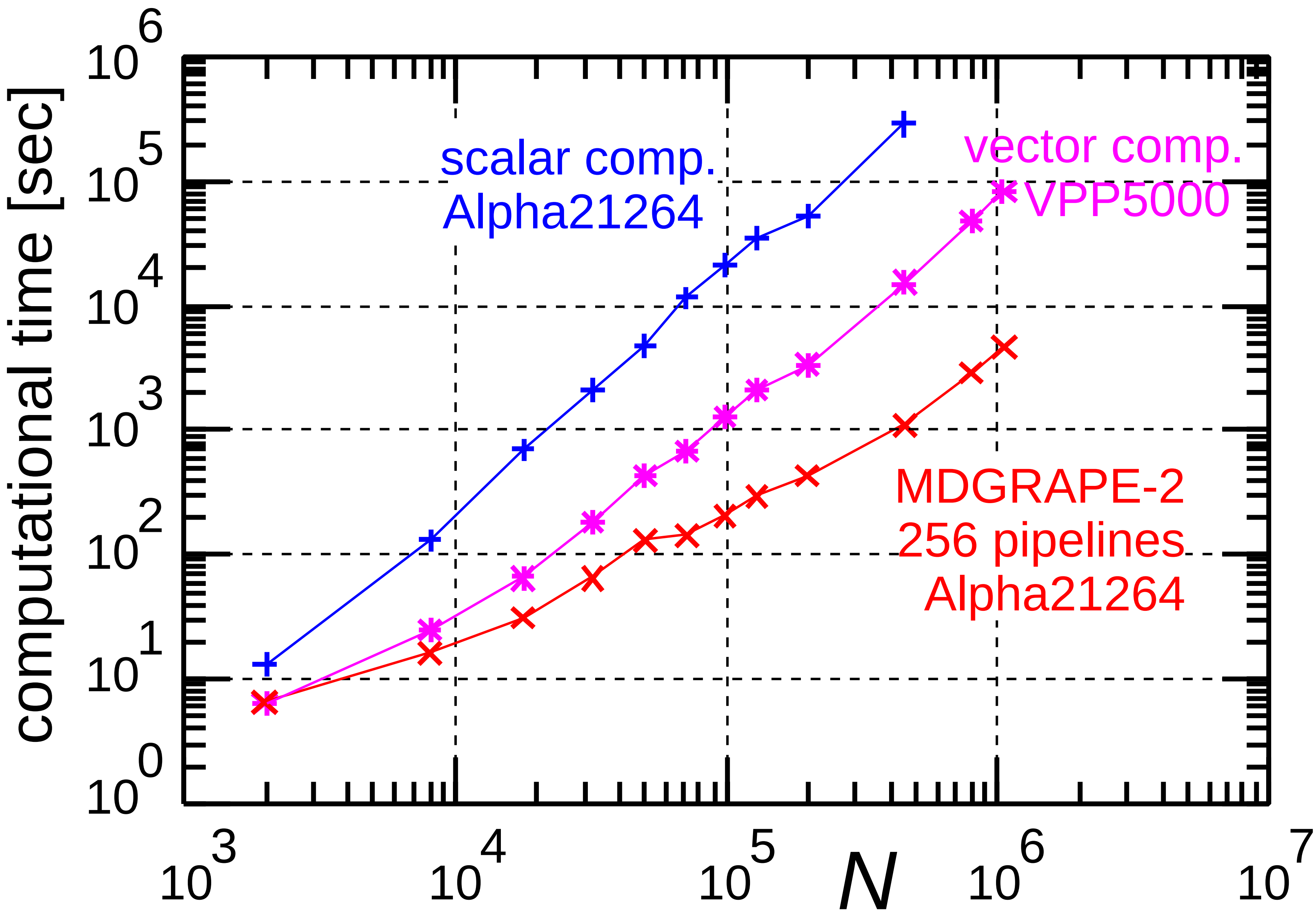
• Benchmark tests

compare

– BIEM on general-purpose computer

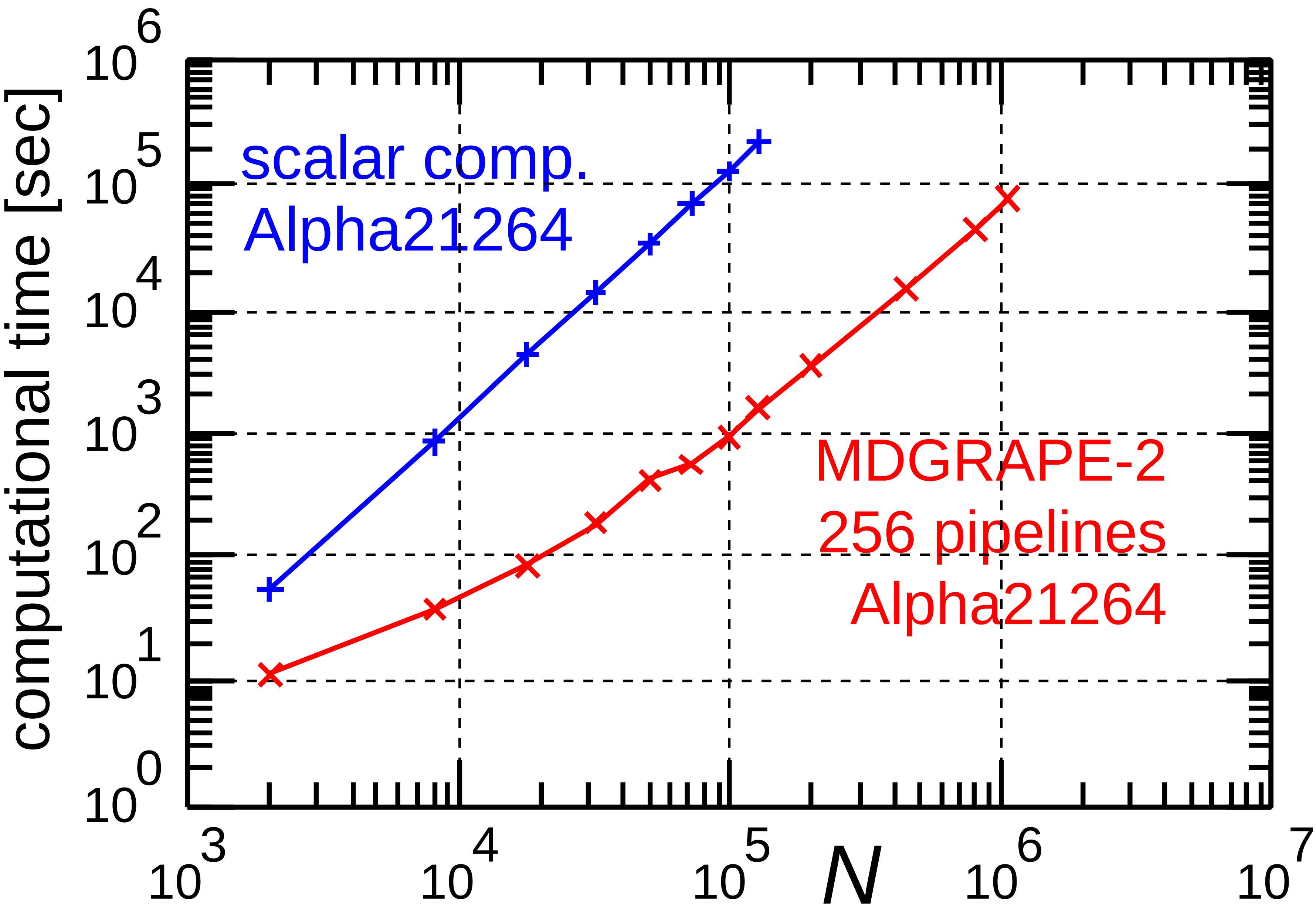
– BIEM on MDGRAPE-2

● Benchmark : Laplace eq. in 3D



10 ∼ 100 times faster ! ; same accuracy

● Benchmark : Helmholtz eq. in 3D



5. Application of MDGRAPE-2 to fast BIEM

MDGRAPE-2 $\xrightarrow{\text{applied successfully}}$ conventional BIEM

$\xrightarrow{\text{next target}}$ fast BIEM

MDGRAPE-2 is directly inapplicable to fast BIEM

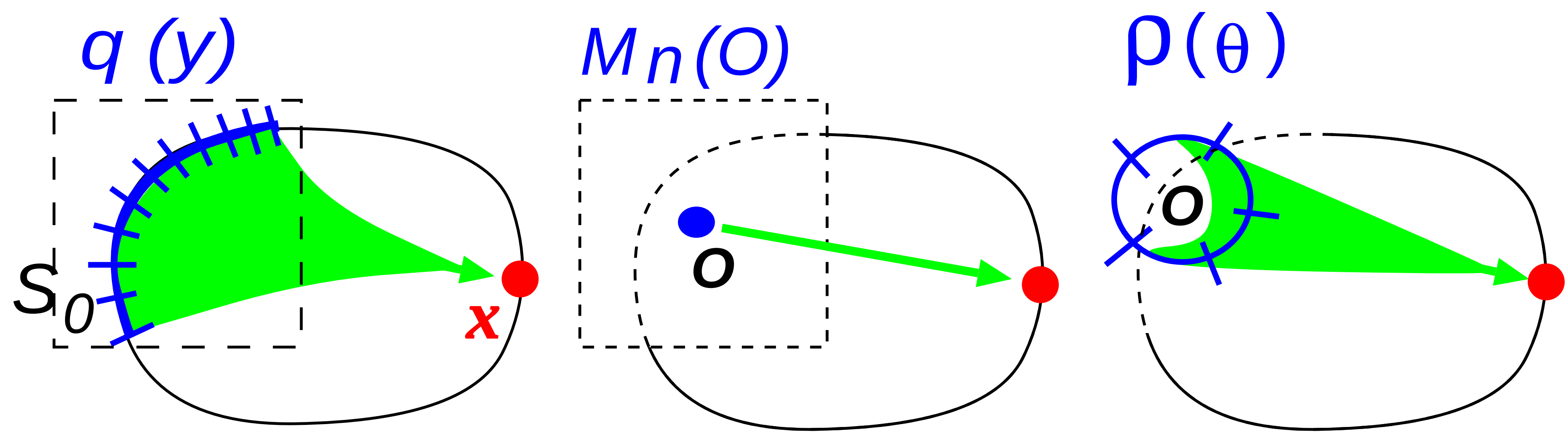
$\downarrow$

we need to modify fast algorithms

● P^{2}M^2 for BIEM

Pseudo-Particle Multipole Method (by Makino and Kawai)

— apply → BIEM for Laplace eq. in 2D



$$\int_{S_0} q(\boldsymbol{y}) \log \frac{1}{\boldsymbol{x}-\boldsymbol{y}} dS_y = \log \frac{1}{\boldsymbol{x}-\boldsymbol{O}} M_0(\boldsymbol{O}) + \sum_{n=1}^{\infty} \frac{a^n}{n(\boldsymbol{x}-\boldsymbol{O})^n} M_n(\boldsymbol{O})$$

$$= \int_0^{2\pi} \rho(\theta) \log \frac{1}{\boldsymbol{x}-\boldsymbol{y}(\theta)} d\theta$$

quad-tree $\longrightarrow$ $O(N \log N)$

6. Conclusion

- MDGRAPE-2 is applied for the acceleration of conventional BIEMs successfully.
- MDGRAPE-2 could accelerate fast BIEM with help of P^2M^2.

• Collaborators

- MDGRAPE-2 developers :

  A.Kawai (Saitama Inst. of Tech.),

  T.Ebisuzaki, T.Narumi, Y.Ohno,

  R.Susukita and M.Taiji (RIKEN)

- BIEM researchers :

  N.Nishimura, K.Yoshida and H.Yoshikawa (Kyoto Univ.),

  T.Ueta (Chiba Univ.),

  S.Kobayashi (Fukui Univ. of Tech.)

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