Stokesian Dynamics: fast multipole method for computer simulations

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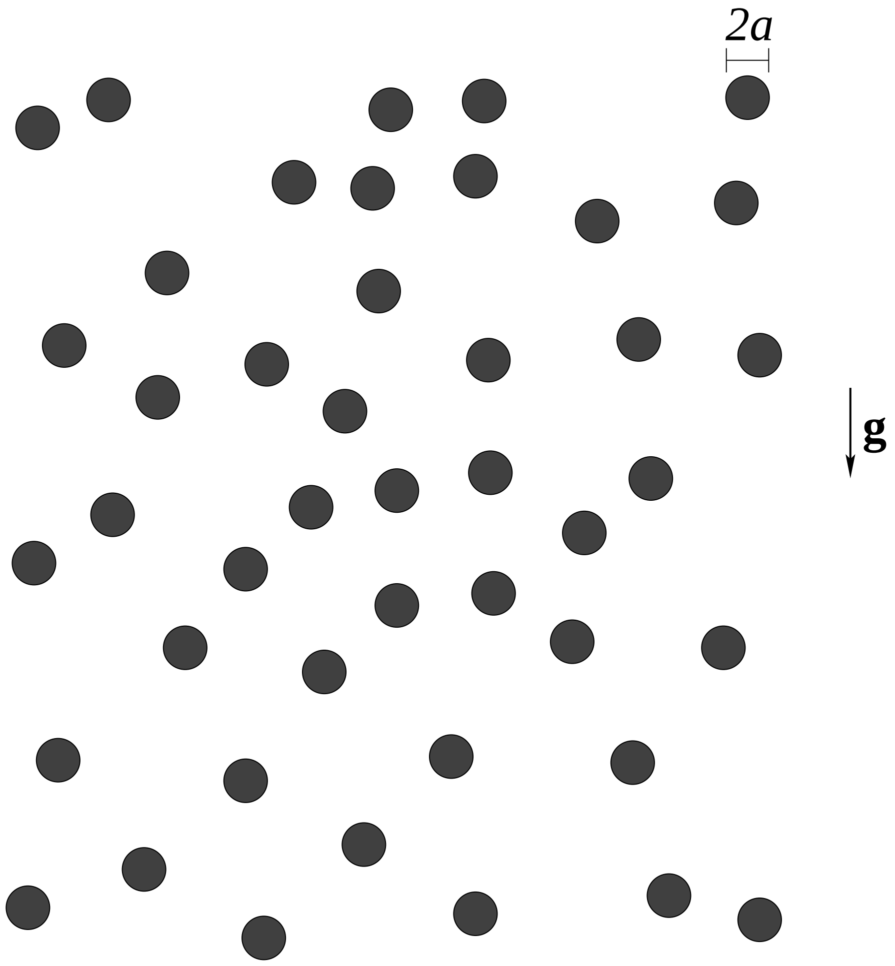
Outline

- Problem statement
- Multipole method

  (Cichocki, Felderhof, Schmitz, Wajnryb, Ekiel-Jeżewska)
- Fast Multipole Method

  (Greengard and Rokhlin)

The system: N hard spheres in an unbounded fluid (η, ρ)



Time scales

convection
$$t_s = \frac{a}{U_0}$$

viscous relaxation
$$t_\eta = a^2 \frac{\rho}{\eta}$$

inertial relaxation
$$t_r = \frac{m}{6\pi\eta a}$$

Brownian diffusion
$$t_d = \frac{a^2}{D}$$

Regime

$$\frac{t_\eta}{t_s} \ll 1, \qquad \frac{t_r}{t_s} \ll 1, \qquad \frac{t_d}{t_s} \gg 1$$

Mobility problem

configuration

$$\begin{pmatrix} \mathbf{U} \\ \boldsymbol{\Omega} \end{pmatrix} = \boldsymbol{\mu}(\mathsf{X}) \begin{pmatrix} \mathbf{F} \\ \mathbf{T} \end{pmatrix}$$

motion

mobility matrix

Governing equations

$$\eta \nabla^2 \mathbf{v} - \nabla p = \mathbf{0} \qquad \nabla \cdot \mathbf{v} = 0$$

Boundary conditions

$$\mathbf{v}(\mathbf{r}) \to \mathbf{0}, \text{ for } |\mathbf{r}| \to \infty$$

$$\mathbf{v}(\mathbf{r}) = \mathbf{u}_i(\mathbf{r}) \equiv \mathbf{U}_i + \mathbf{\Omega}_i \times (\mathbf{r} - \mathbf{R}_i), \quad \mathbf{r} \in S_i, \quad i = 1, \ldots, N$$

Formal solution, induced forces

$$\mathbf{v}(\mathbf{r}) = \sum_{j=1}^{N} \int \mathbf{T}(\mathbf{r} - \mathbf{r}')\mathbf{f}_j(\mathbf{r}')\mathrm{d}\mathbf{r}'; \qquad \mathbf{T}(\mathbf{r}) = \frac{1}{8\pi\eta r}(\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}})$$

System of integral equations for $\mathbf{f}_1, \ldots, \mathbf{f}_N$

$$\begin{aligned}\mathbf{u}_i(\mathbf{r}) &= \int \mathbf{T}(\mathbf{r}-\mathbf{r}') \cdot \mathbf{f}_i(\mathbf{r}')\mathrm{d}\mathbf{r}' + \sum_{j \neq i} \int \mathbf{T}(\mathbf{r}-\mathbf{r}') \cdot \mathbf{f}_j(\mathbf{r}')\mathrm{d}\mathbf{r}' \\ &= [\mathbf{Z}_0^{-1}(i)\mathbf{f}_i](\mathbf{r}) \qquad\qquad + \sum_{j \neq i} [\mathbf{G}(ij)\mathbf{f}_j](\mathbf{r})\end{aligned}$$

For $\mathbf{r} \in S_i$, $i = 1, \ldots, N$

Expansions

Velocity on S_i, $i = 1, \ldots, N$

$$\mathbf{u}_i(\mathbf{r}) = \sum_{lm\sigma} c(ilm\sigma)\mathbf{v}^{+}_{lm\sigma}(\mathbf{r} - \mathbf{R}_i)$$

Green tensor (Perkins and Jones, 1991)

$$\mathbf{T}(\mathbf{r} - \mathbf{r}') = \frac{1}{\eta} \sum_{lm\sigma} \mathbf{v}^{-}_{lm\sigma}(\mathbf{r} - \mathbf{R})[\mathbf{v}^{+}_{lm\sigma}(\mathbf{r}' - \mathbf{R})]^{*}$$

For $|\mathbf{r} - \mathbf{R}| > |\mathbf{r}' - \mathbf{R}|$

$$l = 1, 2, 3, \ldots, \quad |m| \leq l, \quad \sigma = \{0, 1, 2\}$$

Projecting onto multipole functions:

For $i = 1, \ldots, N$

$$c(ilm\sigma) = (lm\sigma|\mathbf{Z}_0^{-1}(i)|l'm'\sigma')f(il'm'\sigma') + \sum_{j \neq i}(lm\sigma|\mathbf{G}(ij)|l'm'\sigma')f(jl'm'\sigma')$$

velocity multipoles

single−particle operator

propagator

force multipoles

$$c(ilm\sigma) = \langle \mathbf{w}^{+}_{lm\sigma}(i)\delta_a|\mathbf{u}_i\rangle \qquad f(ilm\sigma) = \langle \mathbf{v}^{+}_{lm\sigma}(i)|\mathbf{f}_i\rangle$$

$$(i1m0) \rightarrow \mathbf{F}_i, \mathbf{U}_i \qquad (i1m1) \rightarrow \mathbf{T}_i, \mathbf{\Omega}_i$$

Displacement theorems

(Felderhof and Jones, 1988)

For $\mathbf{r} = \mathbf{r}_< + \mathbf{r}_>$ and $|\mathbf{r}_>| > |\mathbf{r}_<|$

$$\mathbf{v}^-_{lm\sigma}(\mathbf{r}) = \eta \sum_{l'm'\sigma'} \mathbf{v}^+_{l'm'\sigma'}(\mathbf{r}_<)(l'm'\sigma'|\mathbf{G}(\mathbf{r}_>)|lm\sigma)$$

$$\mathbf{v}^-_{lm\sigma}(\mathbf{r}) = \sum_{l'm'\sigma'} \mathbf{v}^-_{l'm'\sigma'}(\mathbf{r}_>)(l'm'\sigma'|\mathbf{S}(\mathbf{r}_<)|lm\sigma)$$

Force multipole equations

$$\mathbf{M} \equiv \mathbf{Z}_0^{-1} + \mathbf{G} \qquad \mathbf{c} = \mathbf{M} \cdot \mathbf{f} \qquad \mathbf{f} = \mathbf{M}^{-1} \cdot \mathbf{c}$$

Friction problem

$$\begin{pmatrix} \mathbf{F} \\ \mathbf{T} \end{pmatrix} = \zeta \begin{pmatrix} \mathbf{U} \\ \boldsymbol{\Omega} \end{pmatrix} \qquad \zeta = \mathcal{P}\mathbf{M}\mathcal{P}$$

$\boldsymbol{\zeta}$: resistance matrix, $\mathcal{P}$: projection onto $l = 1; \sigma = (0, 1)$

Truncation ($l \leq L$) and lubrication correction

$$\zeta_L = \mathcal{P}\mathbf{M}_L^{-1}\mathcal{P} + \boldsymbol{\Delta}_L \qquad \zeta = \lim_{L\to\infty} \zeta_L$$

Mobility matrix

$$\boldsymbol{\mu} = \left[\mathcal{P}\mathbf{M}_L^{-1}\mathcal{P} + \boldsymbol{\Delta}_L\right]^{-1}$$

Solution by Cholesky factorization → computational effort $O(N^3)$

Accelarated method ($O(N)$???)

- Iterative method to solve $\mathbf{c} = (\mathbf{Z}_0^{-1} + \mathbf{G}) \cdot \mathbf{f}$
- Fast matrix-vector multiplication → FMM

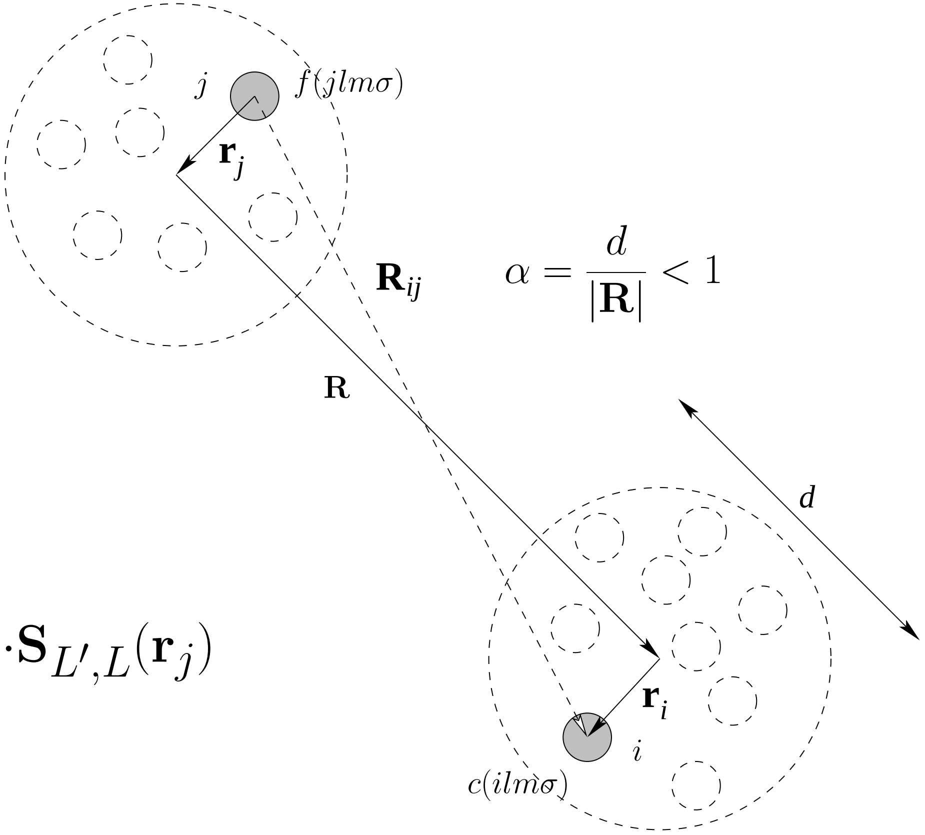
Interactions between well separated groups

Displacement of the propagator

(Cichocki, Ekiel−Jezewska and Wajnryb, 2007)

$$\mathbf{G}(\mathbf{R}) = \mathbf{G}(\mathbf{R}_{>}) \cdot \mathbf{S}(\mathbf{R}_{<})$$

$$\mathbf{G}^{\dagger}(\mathbf{R}) = \mathbf{G}(-\mathbf{R})$$



$$\alpha = \frac{d}{|\mathbf{R}|} < 1$$

Truncation

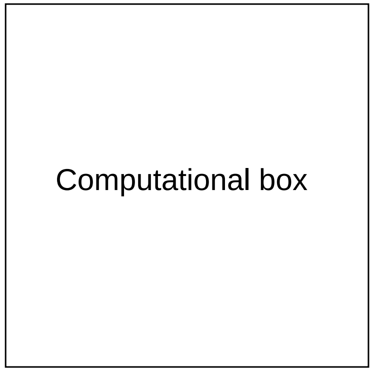
$$\mathbf{G}_L(\mathbf{R}_{ij}) = \mathbf{S}^{\dagger}_{L,L'}(-\mathbf{r}_i) \cdot \mathbf{G}_{L'}(\mathbf{R}) \cdot \mathbf{S}_{L',L}(\mathbf{r}_j)$$

$$L' \geq L$$

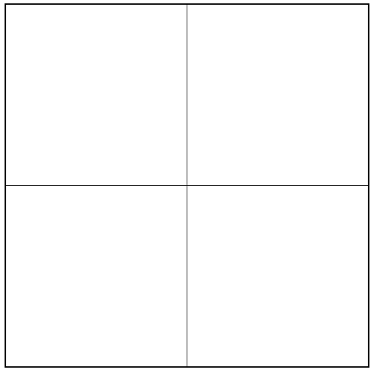
truncation order for groups

Fast Multipole Method (Greengard and Rokhlin, 1987)

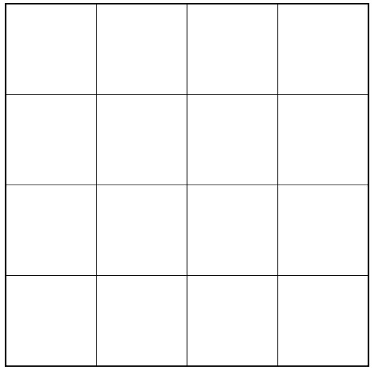
Multilevel partition of the computational domain



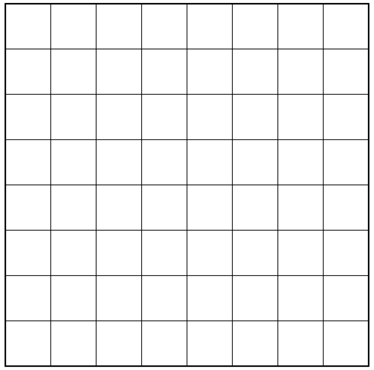
Level 0



Level 1



Level 2

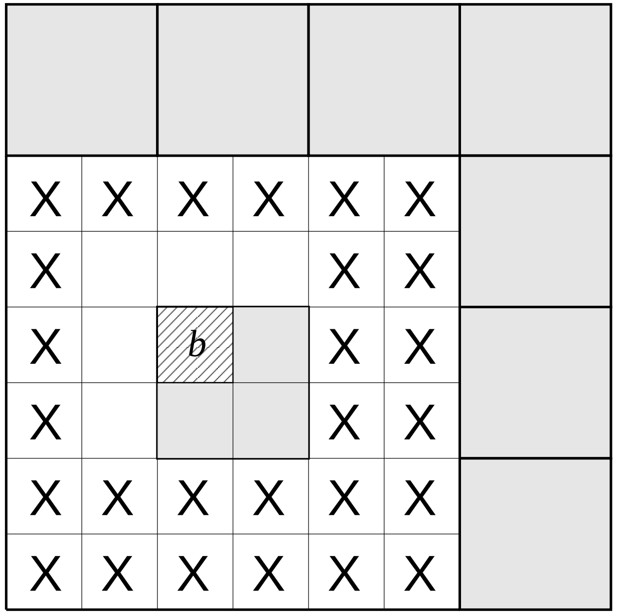


Level 3

Nearest neighbourhood and interaction lists

NN : nearest neighbours
(same level)

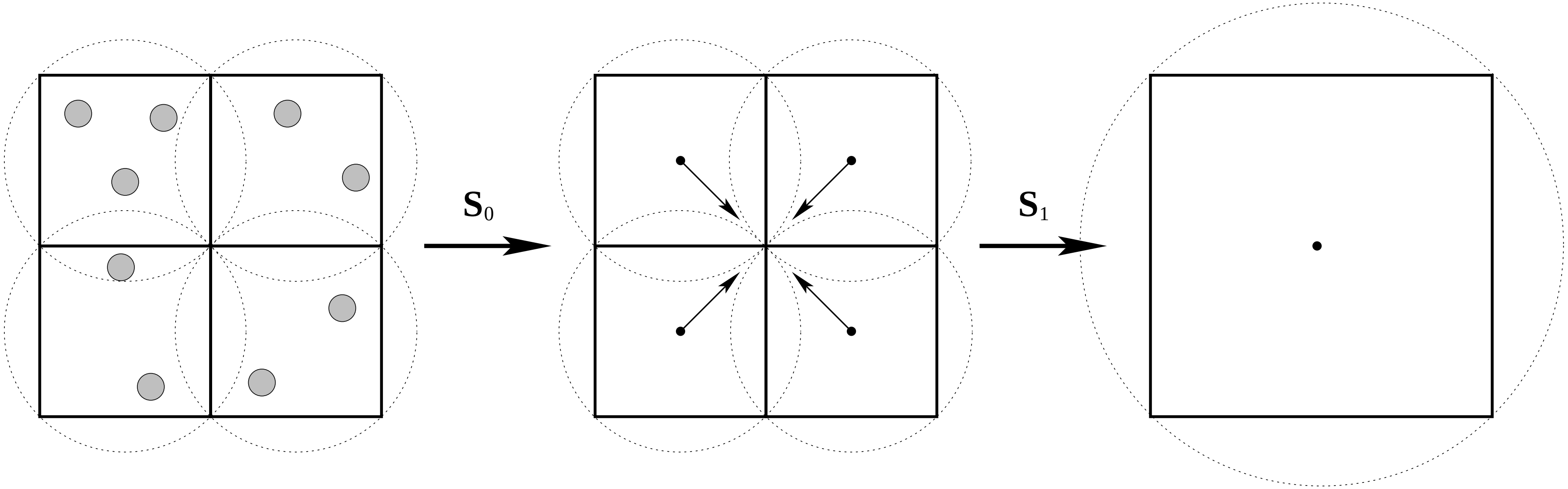
well−separated
boxes



X: interaction list

$\mathcal{N}(n_\ell)$: nearest neighbourhood, $\mathcal{I}(n_\ell)$: interaction list

Collecting moments (upward pass)



$$(n|\mathbf{S}_0|i) = \begin{cases} \mathbf{S}(\mathbf{r}_{ni}) & \text{if } i \in \text{ cell } n \\ \mathbf{0} & \text{otherwise} \end{cases} \qquad (n'|\mathbf{S}_1|n) = \begin{cases} \mathbf{S}(\mathbf{r}_{n'n}) & \text{if } n \text{ is a child of } n' \\ \mathbf{0} & \text{otherwise} \end{cases}$$

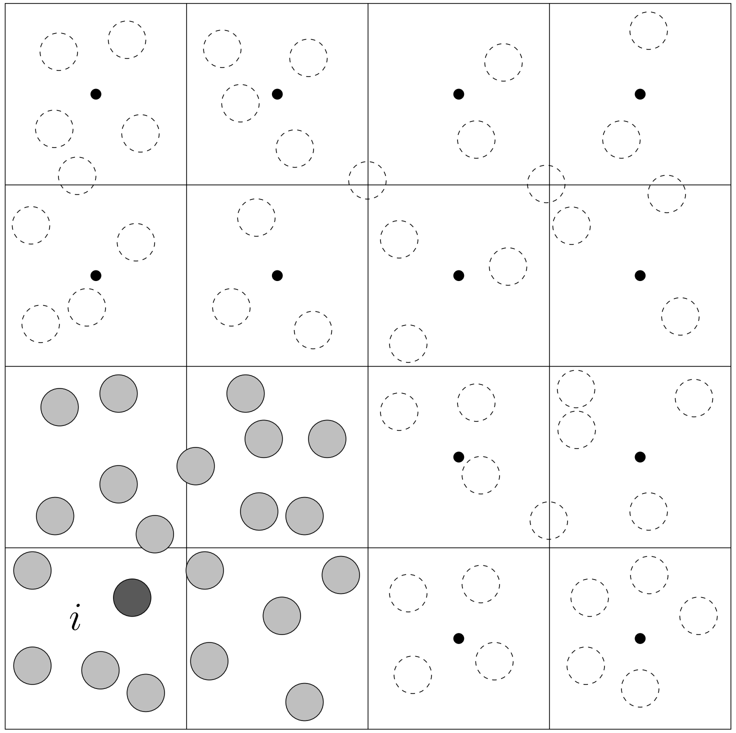
Propagators

Nearest Neighbours

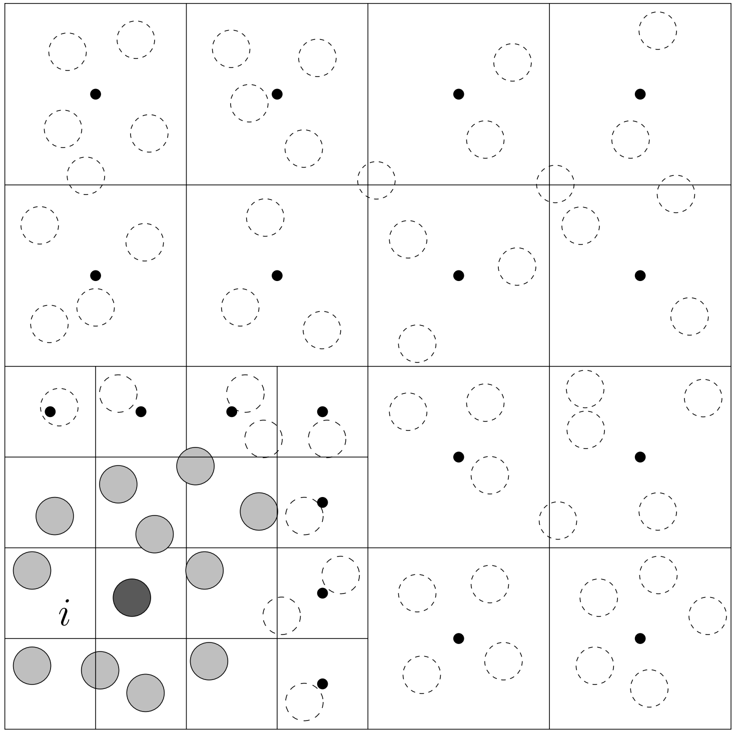
$$(i|\mathbf{G}_{\mathsf{NN}}|j) = \begin{cases} \mathbf{G}(\mathbf{R}_i - \mathbf{R}_j) & \text{if } \mathcal{N}(i) \cap \mathcal{N}(j) \neq \emptyset \\ \\ 0 & \text{otherwise} \end{cases}$$

Well separated cells

$$(n|\mathbf{G}_p|n') = \begin{cases} \mathbf{G}(\mathbf{R}_n - \mathbf{R}_{n'}) & \text{if } \mathcal{I}(n) \cap \mathcal{I}(n') \neq \emptyset \\ \\ 0 & \text{otherwise} \end{cases}$$



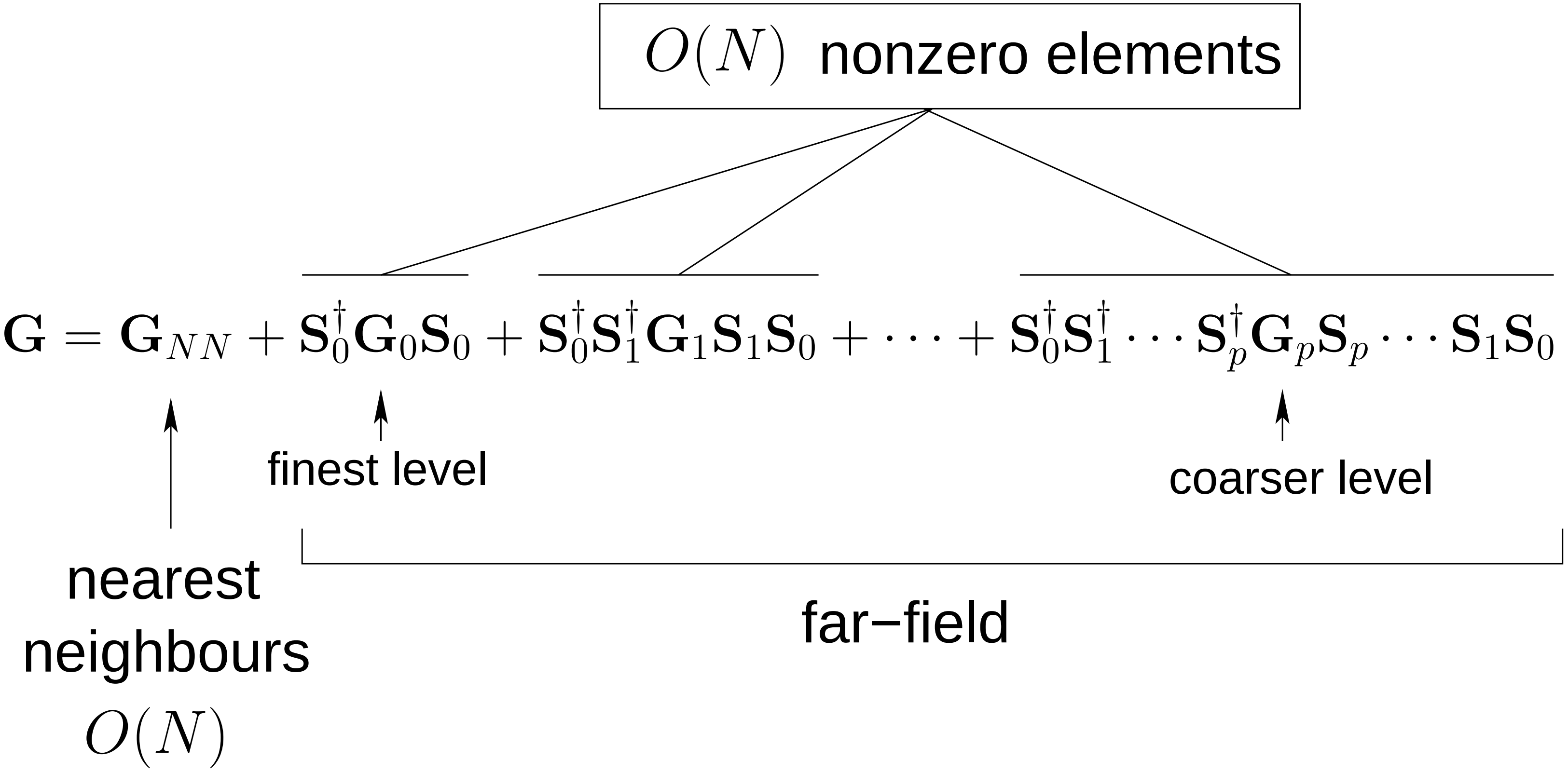
$$\mathbf{G} = \mathbf{G}_{NN} + \mathbf{S}_0^{\dagger}\mathbf{G}_0\mathbf{S}_0$$



$$\mathbf{G} = \mathbf{G}_{NN} + \mathbf{S}_0^{\dagger}[\mathbf{G}_0 + \mathbf{S}_1^{\dagger}\mathbf{G}_1\mathbf{S}_1]\mathbf{S}_0$$

Decomposition of the propagator

For a given multilevel partition, with $p = \ell_{max} - \ell_{min}$



$O(N)$ nonzero elements

$$\mathbf{G} = \mathbf{G}_{NN} + \mathbf{S}_0^\dagger \mathbf{G}_0 \mathbf{S}_0 + \mathbf{S}_0^\dagger \mathbf{S}_1^\dagger \mathbf{G}_1 \mathbf{S}_1 \mathbf{S}_0 + \cdots + \mathbf{S}_0^\dagger \mathbf{S}_1^\dagger \cdots \mathbf{S}_p^\dagger \mathbf{G}_p \mathbf{S}_p \cdots \mathbf{S}_1 \mathbf{S}_0$$

finest level

coarser level

nearest neighbours $O(N)$

far−field

Mobility problem

(Bławzdziewicz and Wajnryb, 2007)

$$(\mathcal{P}\mathbf{M}^{-1}\mathcal{P} + \Delta)\begin{pmatrix} \mathbf{U} \\ \boldsymbol{\Omega} \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{T} \end{pmatrix}, \qquad \mathbf{M} = \mathbf{Z}_0^{-1} + \mathbf{G}$$

$$\mathcal{U}_{\mathcal{P}} \equiv \begin{pmatrix} \mathbf{U} \\ \boldsymbol{\Omega} \end{pmatrix} \qquad \mathcal{F}_{\mathcal{P}} \equiv \begin{pmatrix} \mathbf{F} \\ \mathbf{T} \end{pmatrix} \qquad \mathcal{F}_h : \text{ higher order force moments}$$

Expanded system

$$\left[1 + \mathbf{M}\begin{pmatrix} \Delta & 0 \\ 0 & 0 \end{pmatrix}\right]\begin{pmatrix} \mathcal{U}_{\mathcal{P}} \\ 0 \end{pmatrix} = \mathbf{M}\begin{pmatrix} \mathcal{F}_{\mathcal{P}} \\ \mathcal{F}_h \end{pmatrix}$$

$\mathcal{F}_{\mathcal{P}}$: known

$\mathcal{U}_{\mathcal{P}}, \mathcal{F}_h$: unknowns

Final system

$$\begin{bmatrix} \mathbf{M}_{\mathcal{P}\mathcal{P}} + \mathbf{M}_{\mathcal{P}\mathcal{P}} \Delta \mathbf{M}_{\mathcal{P}\mathcal{P}} & \mathbf{M}_{\mathcal{P}\mathcal{P}} \Delta \mathbf{M}_{\mathcal{P}h} \\ \mathbf{M}_{h\mathcal{P}} \Delta \mathbf{M}_{\mathcal{P}\mathcal{P}} & -(\mathbf{M}_{hh} - \mathbf{M}_{h\mathcal{P}} \Delta \mathbf{M}_{\mathcal{P}h}) \end{bmatrix} \begin{bmatrix} \mathcal{F}'_{\mathcal{P}} \\ \mathcal{F}_h \end{bmatrix} = \mathbf{M} \begin{bmatrix} \mathcal{F}_{\mathcal{P}} \\ 0 \end{bmatrix}$$

Solved iteratively using the Symmetric Quasi-Minimal Residual Method (SQMR)

Solution

$$\mathcal{U}_{\mathcal{P}} = \begin{pmatrix} \mathbf{U} \\ \mathbf{\Omega} \end{pmatrix} = \mathbf{M}_{\mathcal{P}\mathcal{P}} \mathcal{F}'_{\mathcal{P}} + \mathbf{M}_{\mathcal{P}h} \mathcal{F}_h$$

Comparison (for $\phi = 0.1$, periodic boundary conditions)

$$\mathbf{F}_1, \ldots, \mathbf{F}_N = (\ 1\ 0\ 0) \quad \rightarrow \quad \mathbf{U} = (\mathbf{U}_1, \ldots, \mathbf{U}_N)$$

N	L	L'	CPU time ($O(N^3)$) (s)	CPU time (FMM) (s)	Relative error in **U**
64	3	3	52	17	1.75×10^{-2}
		4		28	6.47×10^{-3}
		5		51	3.07×10^{-3}
128	3	3	407	63	1.64×10^{-2}
		4		82	6.03×10^{-3}
		5		117	2.88×10^{-3}