Neutral Territory Decomposition for Parallel MD

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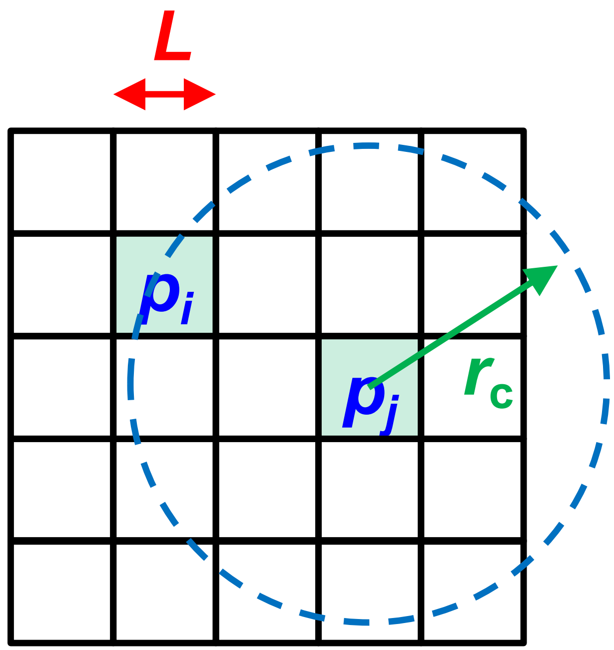
D. E. Shaw, A fast, scalable method for the parallel evaluation of distance-limited pairwise particle interactions, *J. Comput. Chem*. **26**, 1318 ('05)

Fine Granularity

Number of atoms per process (N/P) ~ 1

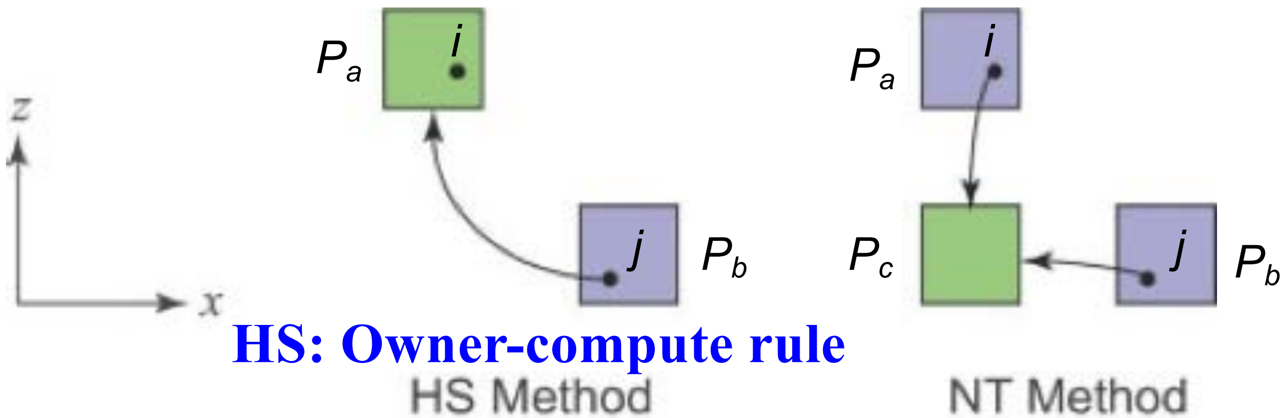
***cf.* Biomolecular simulations**



spatial subsystem length (L) << interaction cutoff (r_c)

Spatial (Half-Shell) *vs.* NT Decompositions

Locus of interaction — who does what (2-dimensional example)



HS: Owner-compute rule

NT = hybrid spatial (data) & force (computation) decomposition with well-designed order/layout

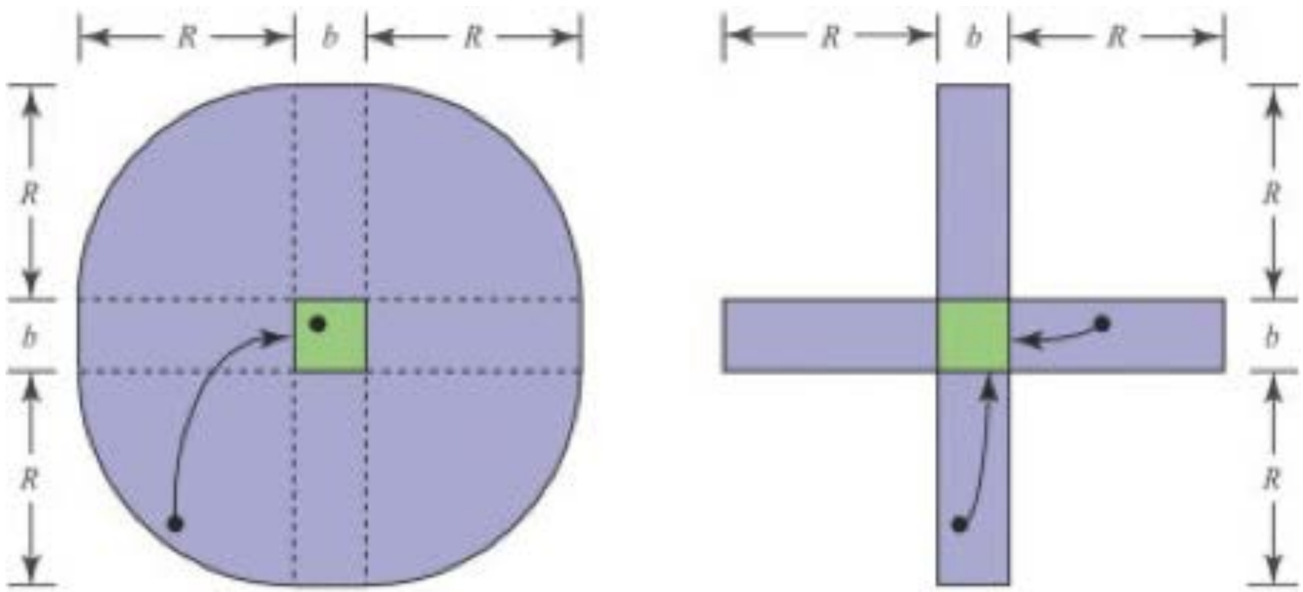
Import regions or communication volume (2-dimensional example)

HS

$4bR+\pi R^2$

$\rightarrow$const.

$(b\rightarrow 0)$



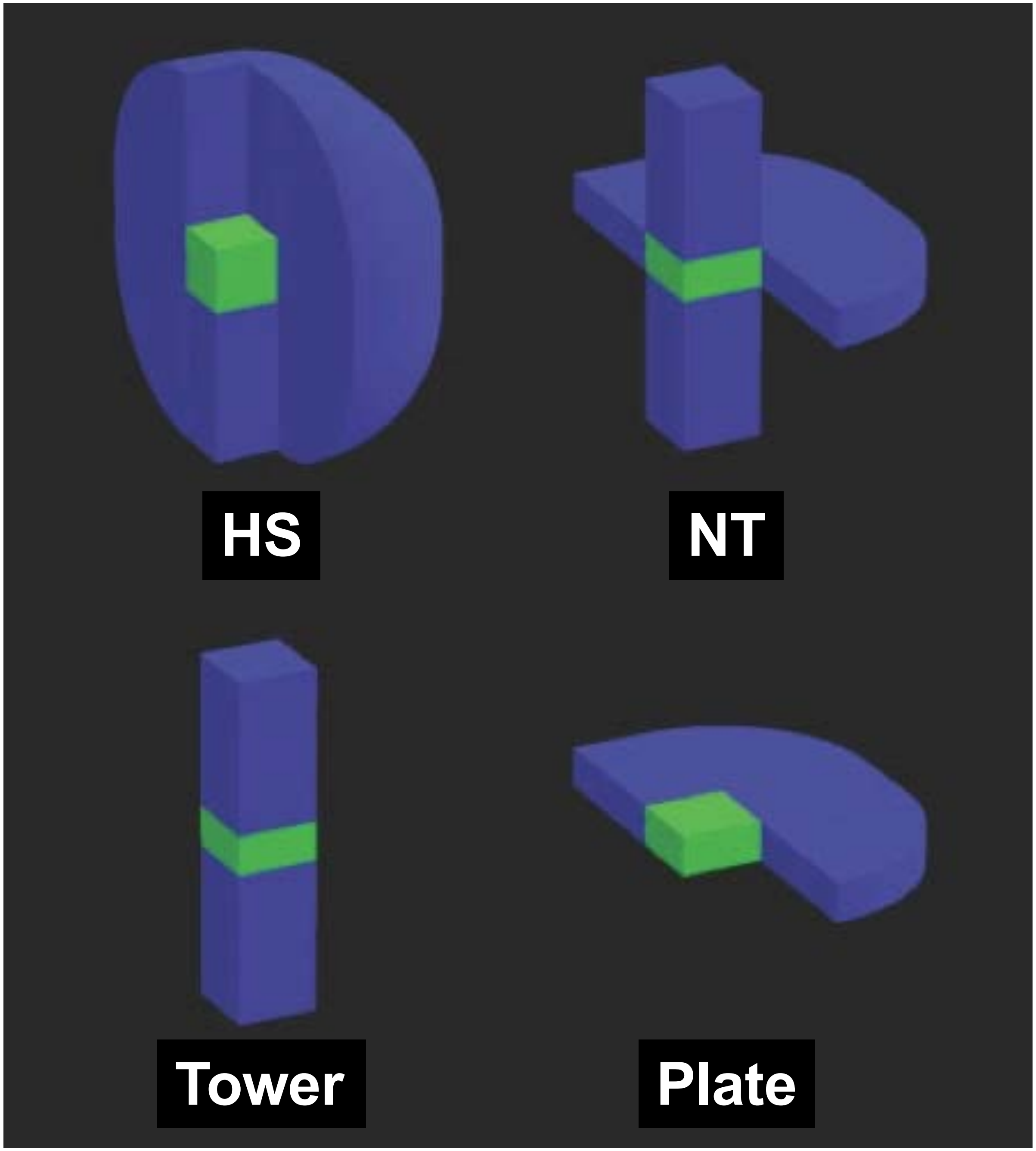
NT

$4bR$

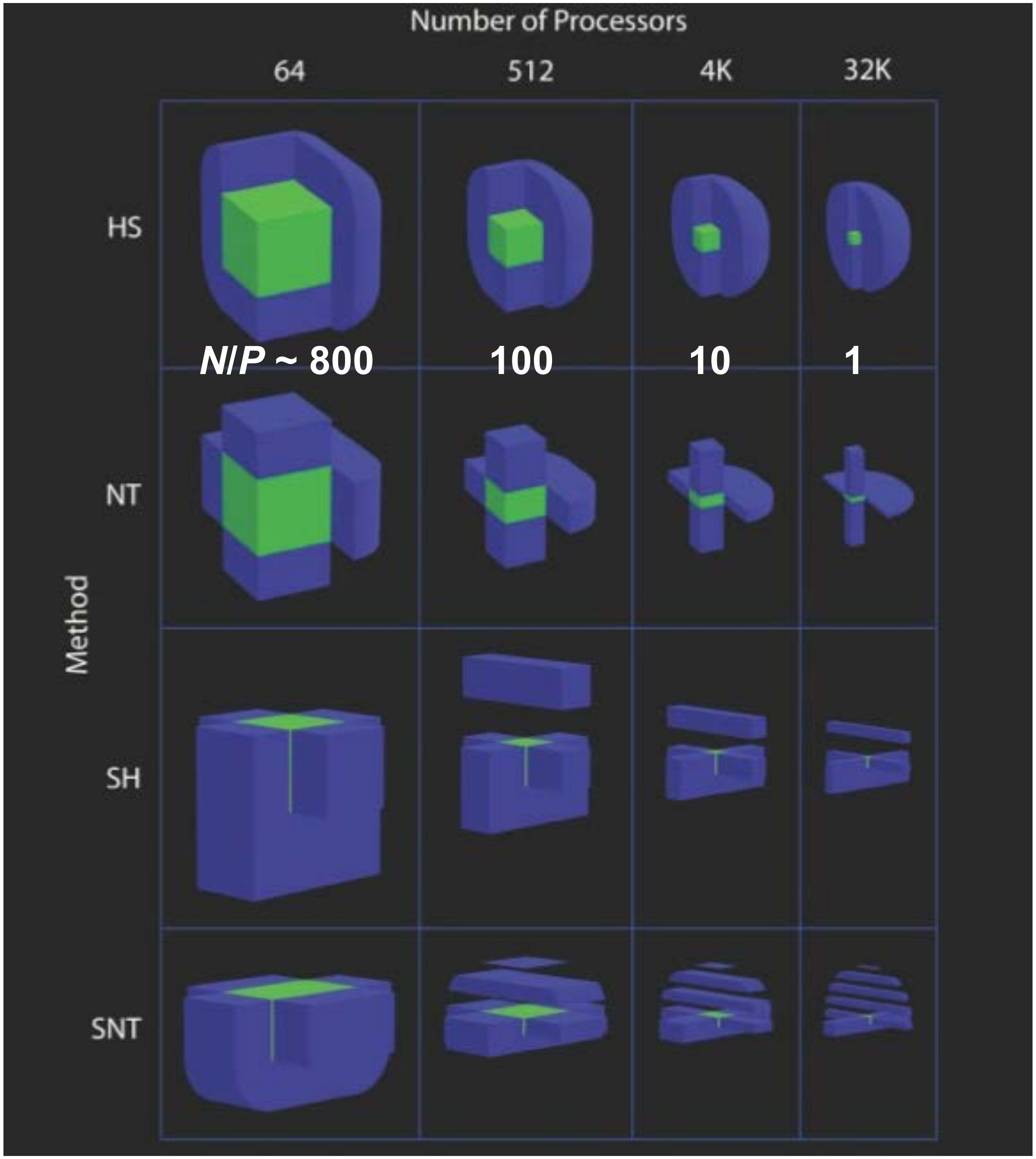
$\rightarrow 0$

$(b\rightarrow 0)$

3D Import Regions



Scaling of Import Regions

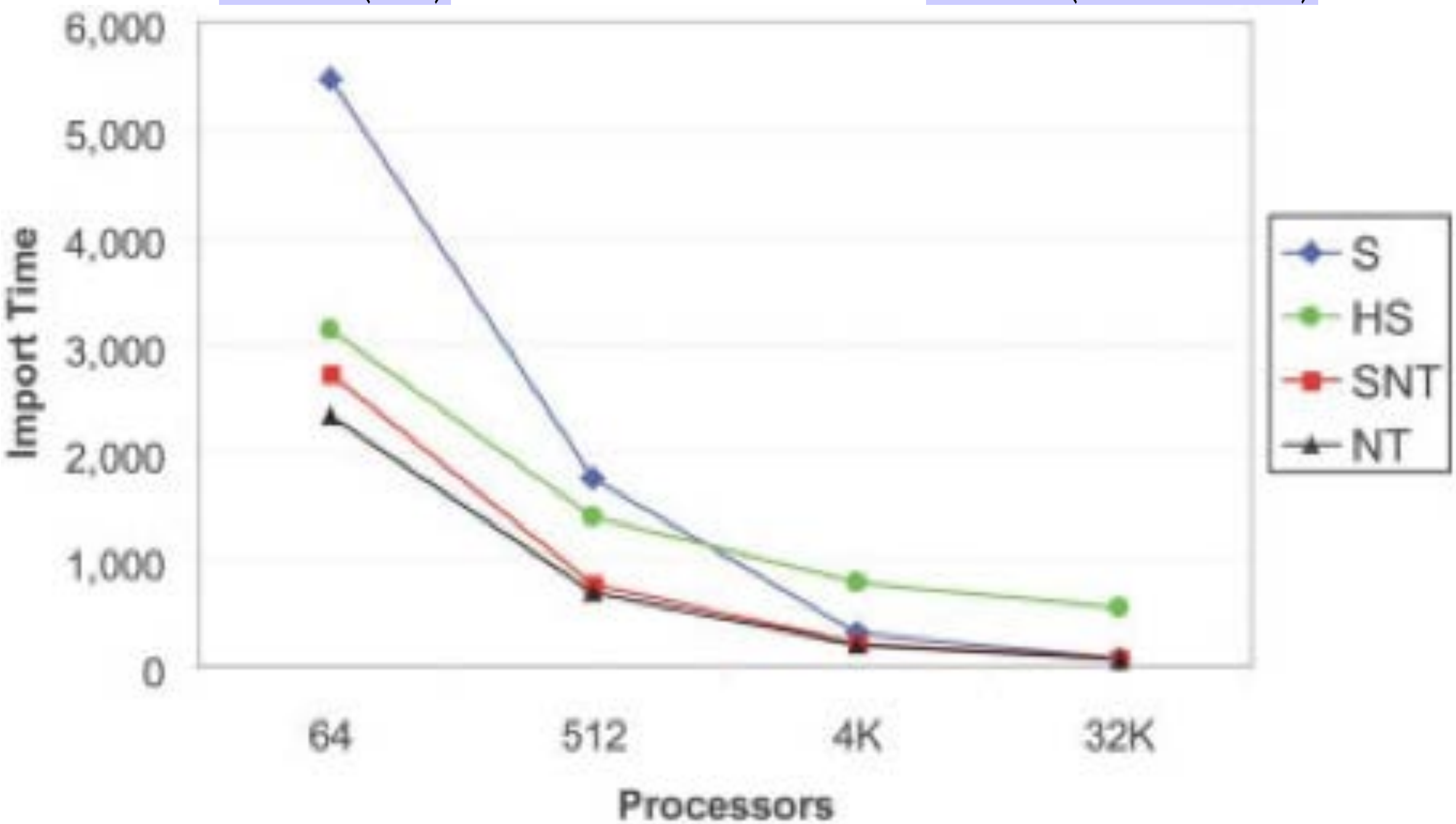


Marc Snir

Scaling of the Volume of Import Regions

HS decomposition $V_i = O\left(R^3\right)$

NT decomposition $V_i = O\left(R^{3/2} p^{-1/2}\right)$



Communication time

$$T_{\text{comm}} = \underbrace{t_{\text{latency}}}_{\text{ns} \sim \text{many } \mu\text{s}} \overbrace{N_{\text{message}}}^{\text{\# of messages}} + \frac{1}{\underbrace{b_{\text{bandwidth}}}_{\text{GB/s}}} \overbrace{V_{\text{message}}}^{\text{volume (Bytes) of messages}}$$

Combine NT with ...

Cache-oblivious recursive blocking?

Cache-Oblivious Algorithms

EXTENDED ABSTRACT SUBMITTED FOR PUBLICATION. FOCS99

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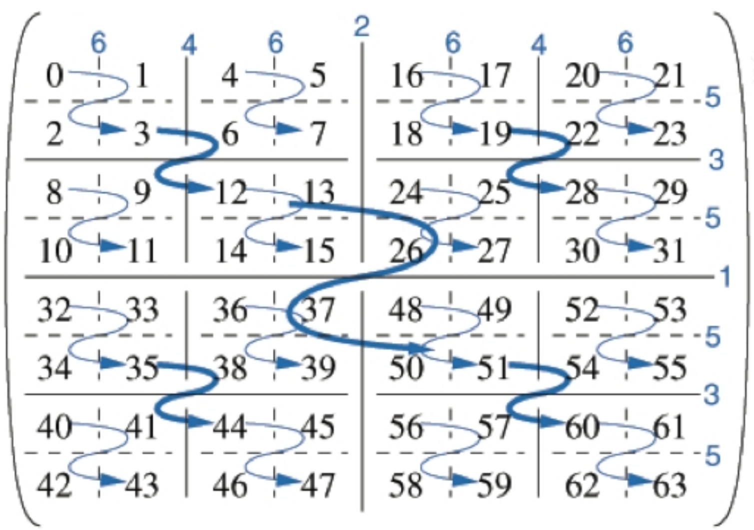
Recursive Blocked Algorithms and Hybrid Data Structures for Dense Matrix Library Software*



Erik Elmroth[†]
Fred Gustavson[‡]
Isak Jonsson[†]
Bo Kågström[†]

Combine NT with ...

Optimal data/computation layout (on Cell, GPU, multicore,...)?

Improving Memory Hierarchy Performance for Irregular Applications*

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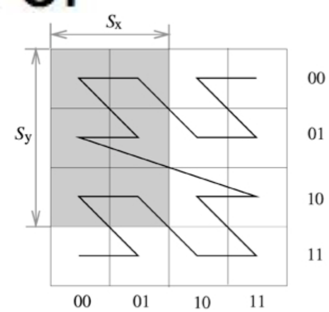
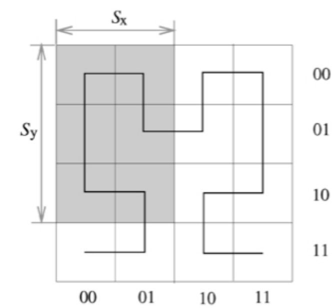
ISC99

IEEE TRANSACTIONS ON KNOWLEDGE AND DATA ENGINEERING, VOL. 13, NO. 1, JANUARY/FEBRUARY 2001

Analysis of the Clustering Properties of the Hilbert Space-Filling Curve

Bongki Moon, H.V. Jagadish, Christos Faloutsos, *Member*, *IEEE*, and Joel H. Saltz, *Member*, *IEEE*





Morton or Hilbert?

Metrics and Models for Reordering Transformations

MSP04

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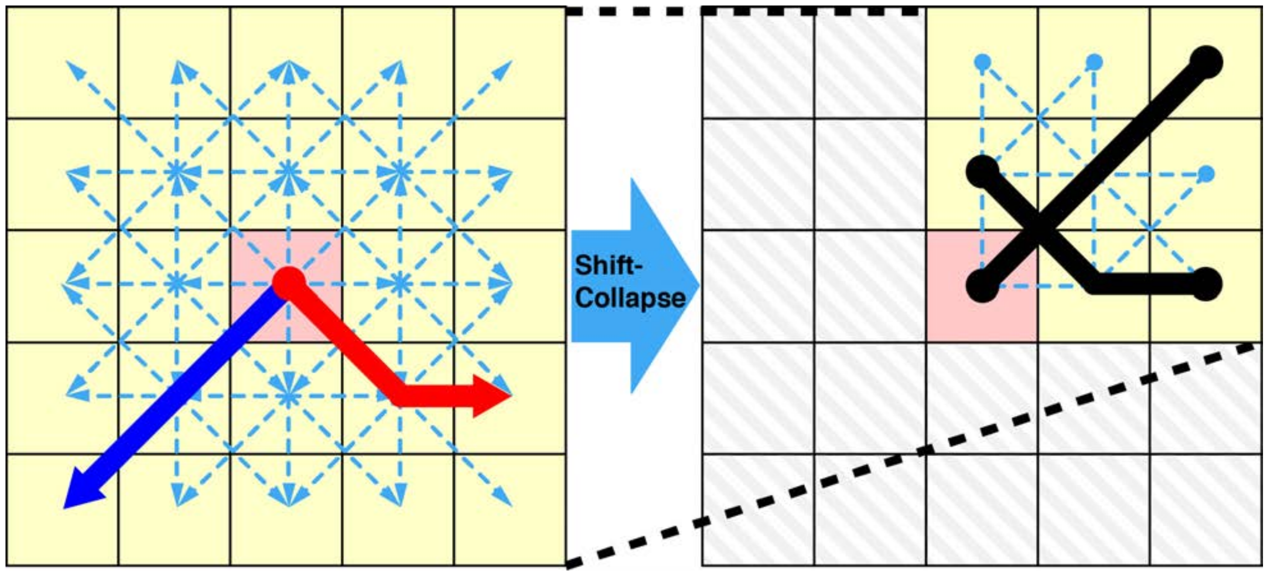
Hypergraph

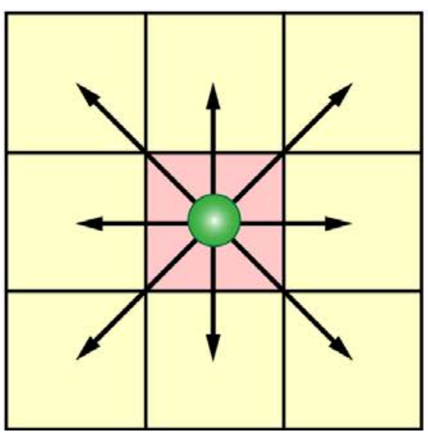
G.M. Morton, "A computer oriented geodetic data base & a new technique in file sequencing," *IBM Tech. Report* ('66)

Shift-Collapse (SC) Algorithm

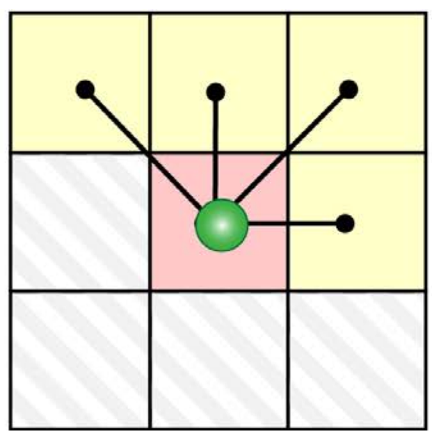
- **Generalization of Shaw's eighth-cell method (non-owner-compute method on high-latency cluster) for pair computation to general dynamic range-limited *n*-tuples**



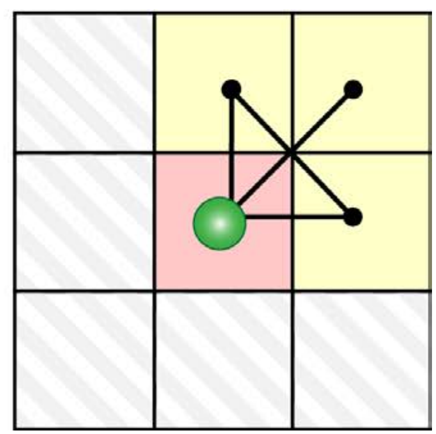
M. Kunaseth *et al*., *IEEE/ACM Supercomputing* (*SC13*)



Full-shell (FS) method
[*e.g*. Rappaport, '88]



Half-shell (HS) method
[*e.g*. Rappaport, '88]



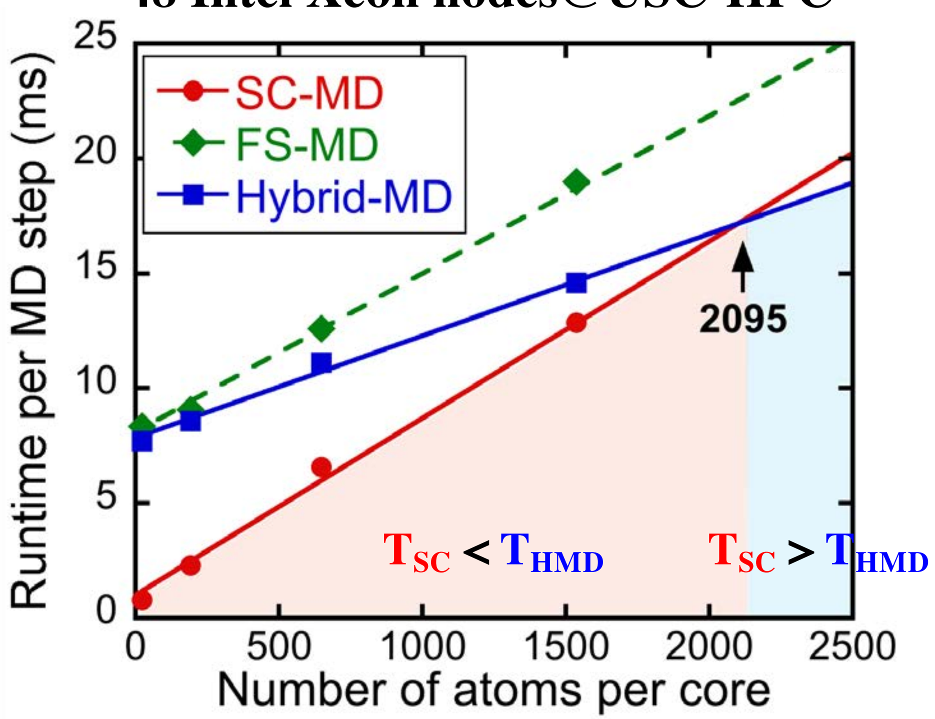
Eighth-shell (ES) method
[Bower *et al*., '06]

Shift-Collapse (SC) Performance

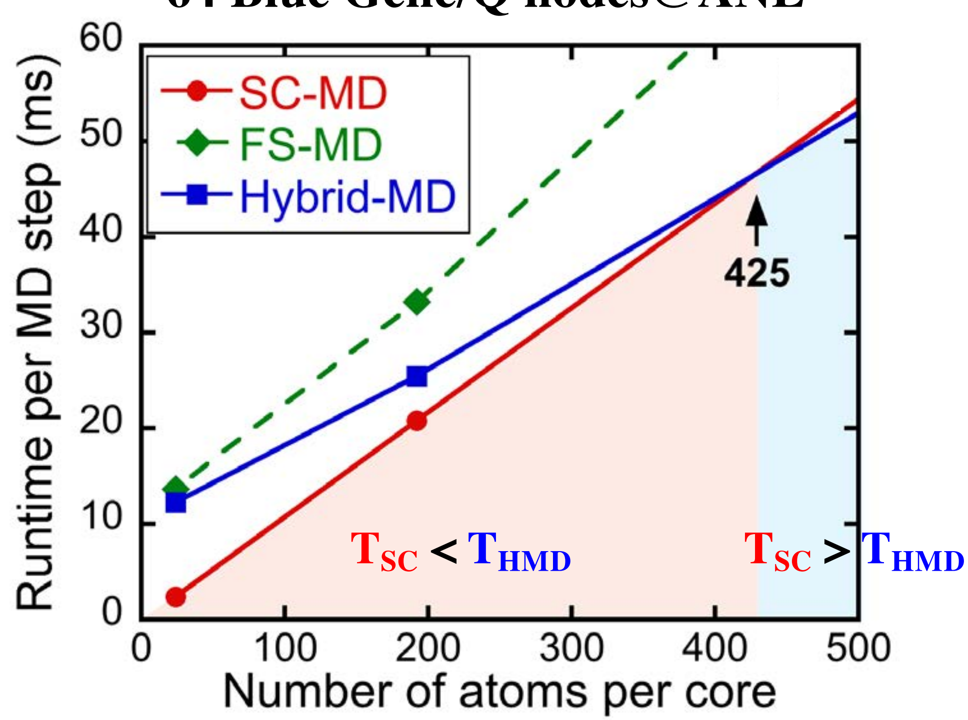
Runtime comparison on 48 Intel-Xeon nodes and 64 Blue Gene/Q nodes

- **SC-MD is always faster than FS-MD**
- **At the smallest grain, SC-MD is 9.7- and 5.1-fold speedups over the state-of-the-art hybrid linked-cell & neighbor list code**
- **Crossover of optimal algorithm from SC-MD to hybrid MD at larger granularity (*i.e.* *N*/*P* > 2,095 on Intel Xeon and *N*/*P* > 425)**

48 Intel Xeon nodes@USC-HPC



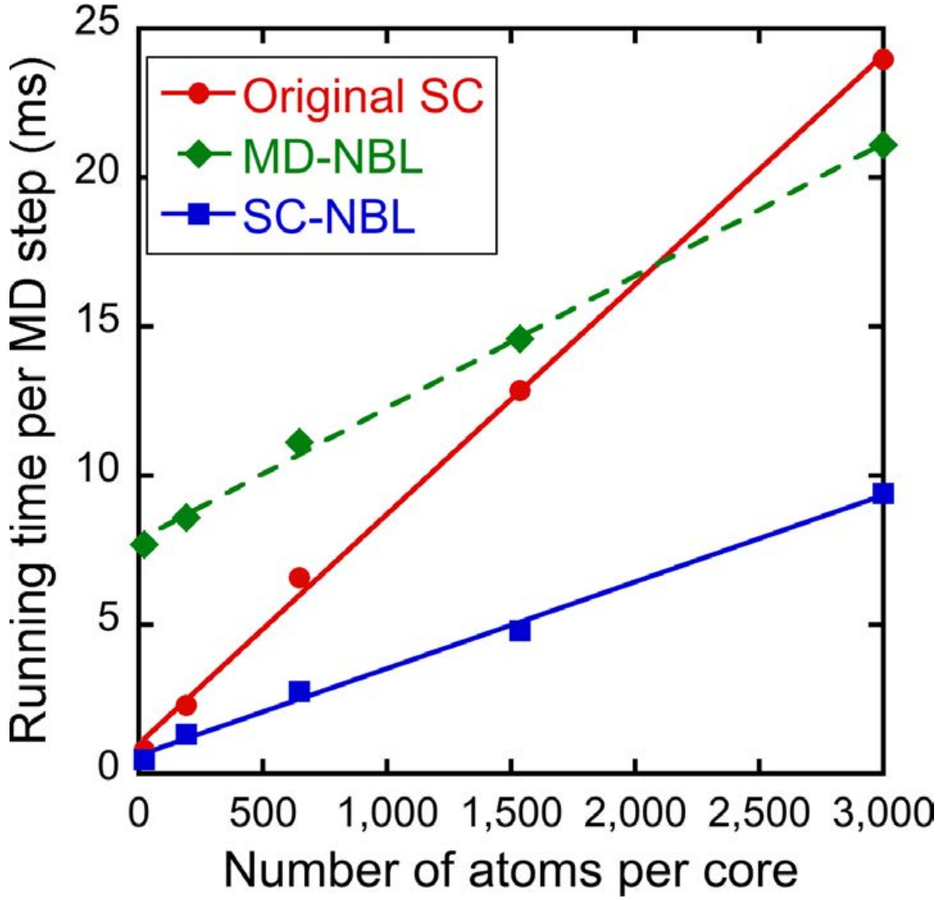
64 Blue Gene/Q nodes@ANL



M. Kunaseth *et al*., *IEEE/ACM Supercomputing* (*SC13*)

Shift-Collapse on Neighbor List (SC-NBL)

- **Apply shift-collapse operations to the hybrid linked-cell & neighbor list code (best of both)**



[Shift/collapse on neighbor list (SC-NBL): fast evaluation of dynamic many-body potentials in molecular dynamics simulations](), M. Kunaseth, S. Hannongbua, & A. Nakano, *Comput. Phys. Commun.* **235**, 88 (2019)

Challenge: Expose massive data parallelism for SC on graphics processing unit (GPU)