

Neutral Territory Decomposition for Parallel MD

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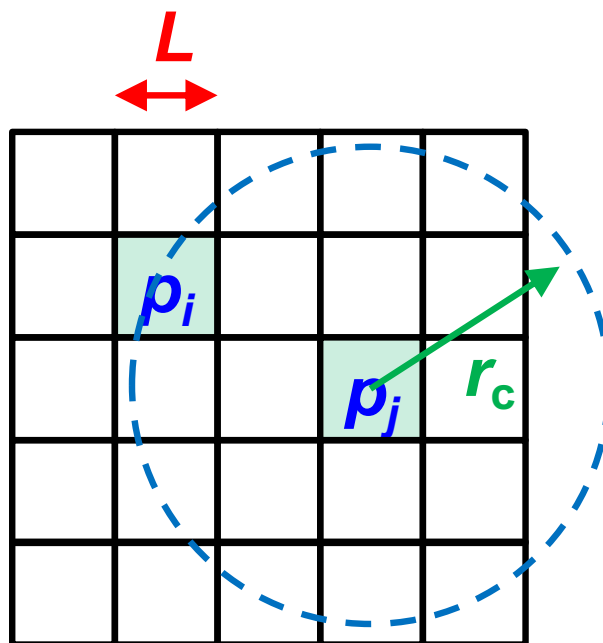
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D. E. Shaw, [A fast, scalable method for the parallel evaluation of distance-limited pairwise particle interactions](#), *J. Comput. Chem.* **26**, 1318 ('05)



Fine Granularity

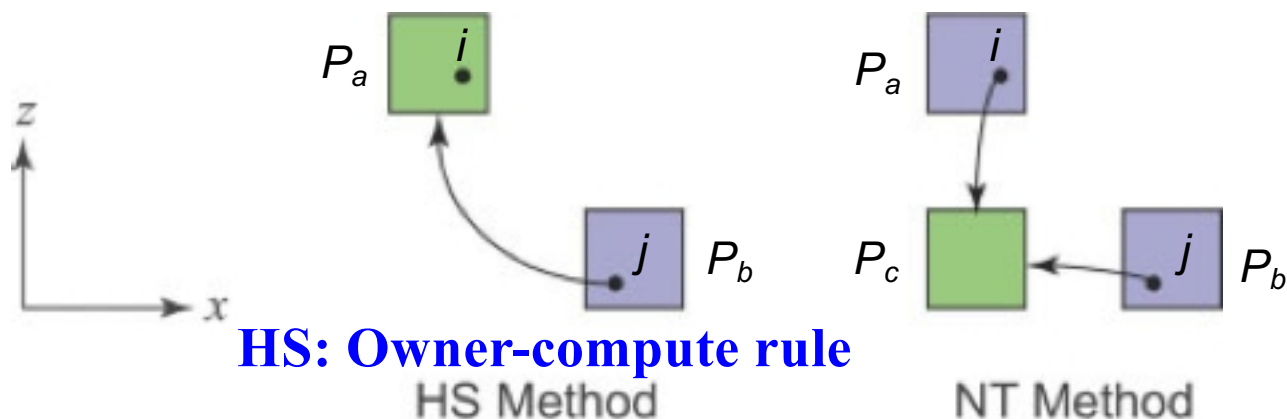
Number of atoms per process (N/P) ~ 1
cf. Biomolecular simulations



spatial subsystem length (L) \ll interaction cutoff (r_c)

Spatial (Half-Shell) vs. NT Decompositions

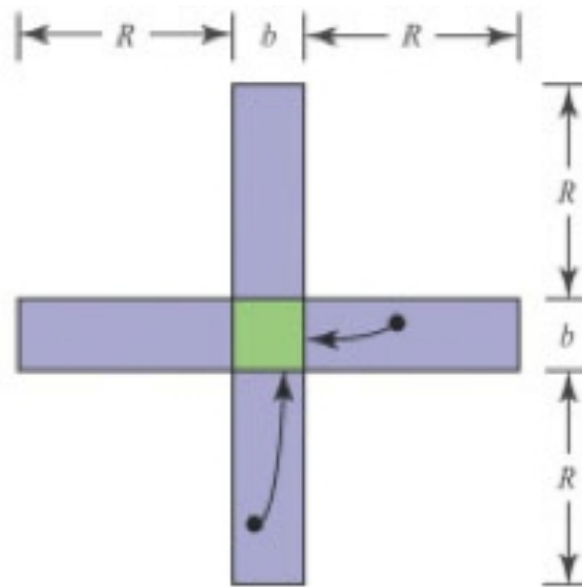
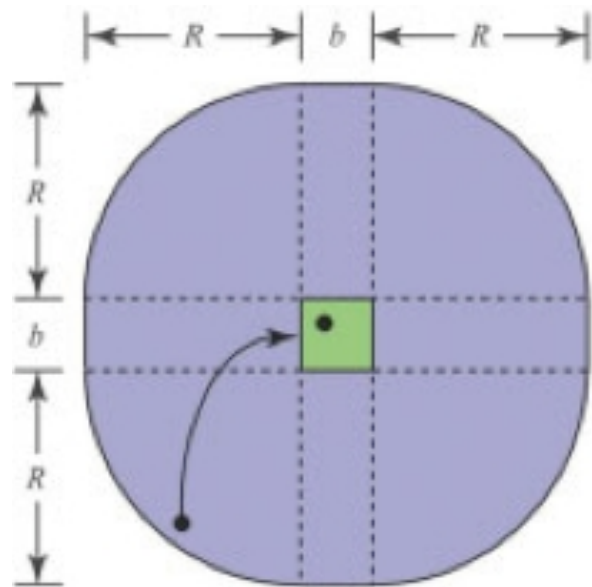
Locus of interaction — who does what (2-dimensional example)



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

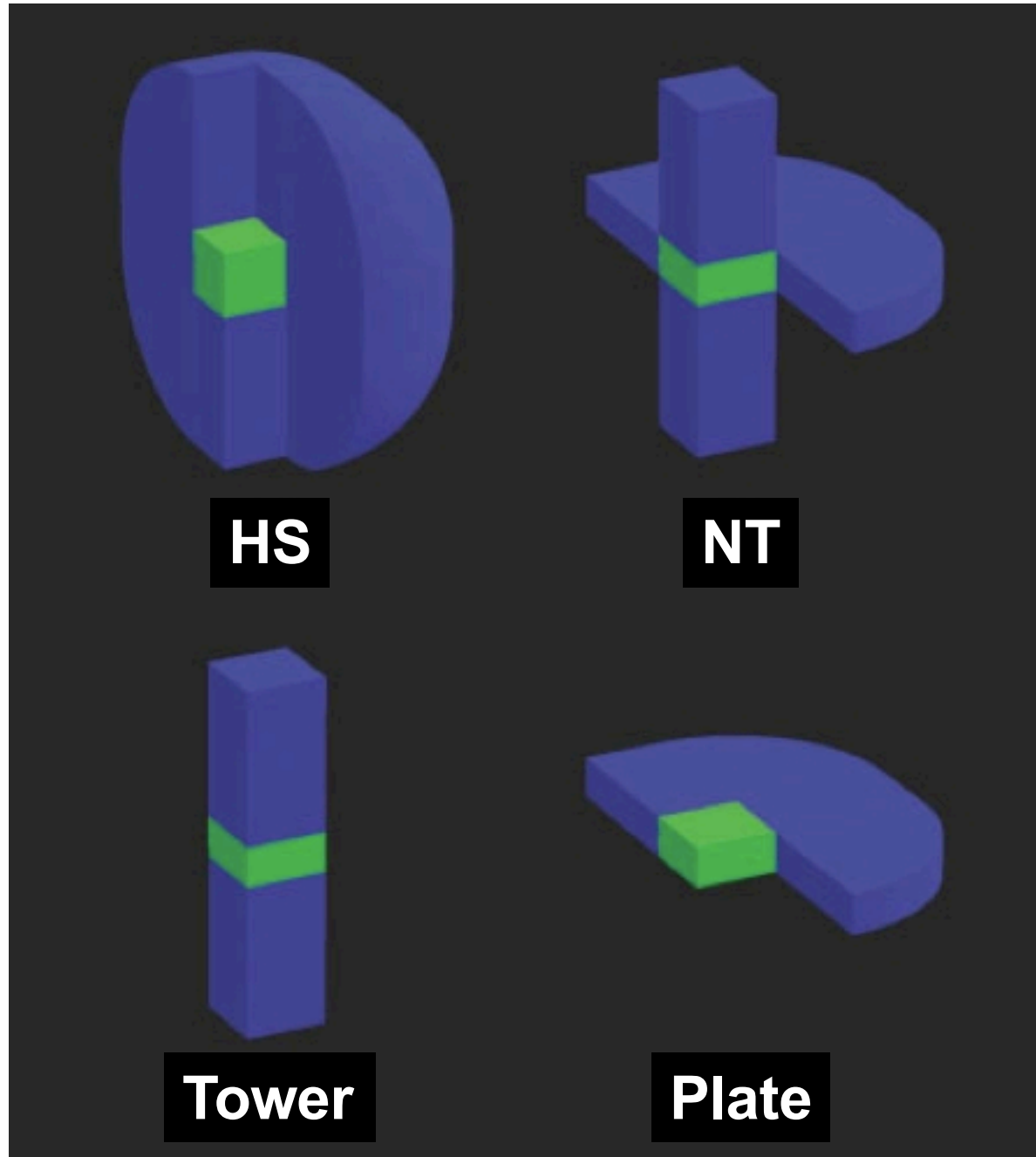
Import regions or communication volume (2-dimensional example)

HS
 $4bR + \pi R^2$
 $\rightarrow \text{const.}$
 $(b \rightarrow 0)$

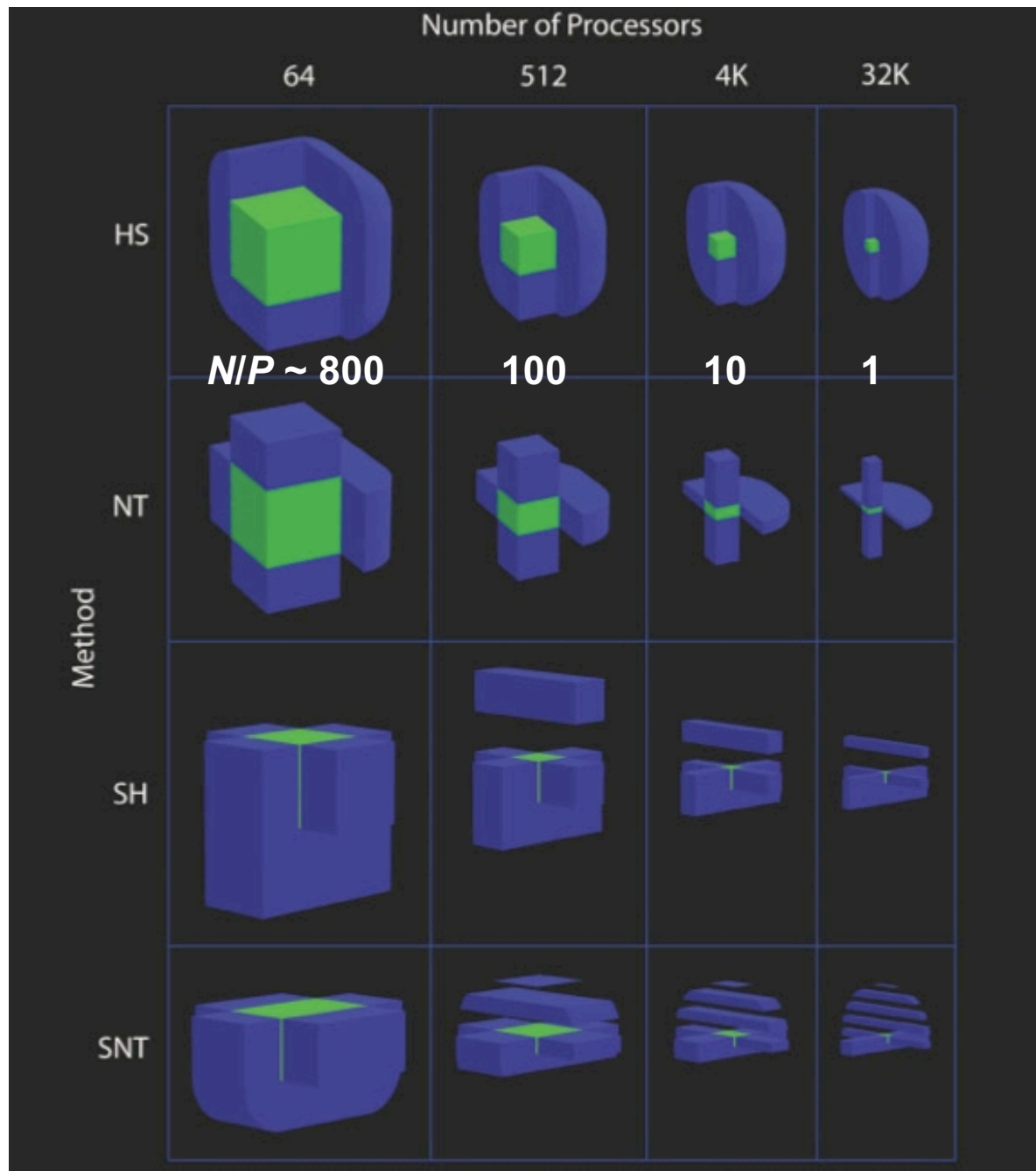


NT
 $4bR$
 $\rightarrow 0$
 $(b \rightarrow 0)$

3D Import Regions



Scaling of Import Regions



Marc Snir

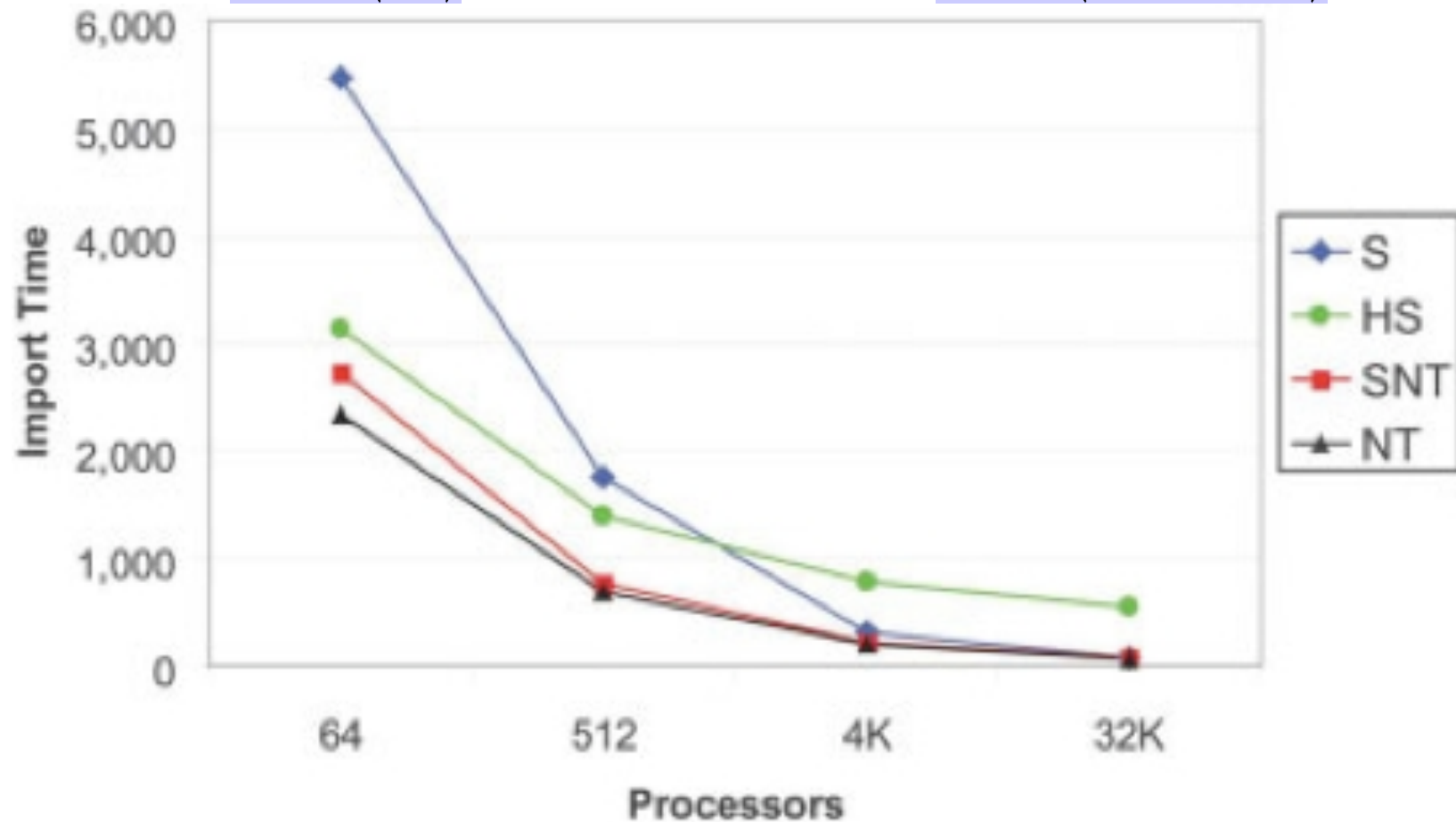
Scaling of the Volume of Import Regions

HS decomposition

$$V_i = O(R^3)$$

NT decomposition

$$V_i = O(R^{3/2} p^{-1/2})$$



Communication time

$$T_{\text{comm}} = t_{\text{latency}} \overset{\text{\# of messages}}{N_{\text{message}}} + \frac{1}{b_{\text{bandwidth}}} \overset{\text{volume (Bytes) of messages}}{V_{\text{message}}}$$

ns ~ many μ s GB/s

Combine NT with ...

Cache-oblivious recursive blocking?

Cache-Oblivious Algorithms

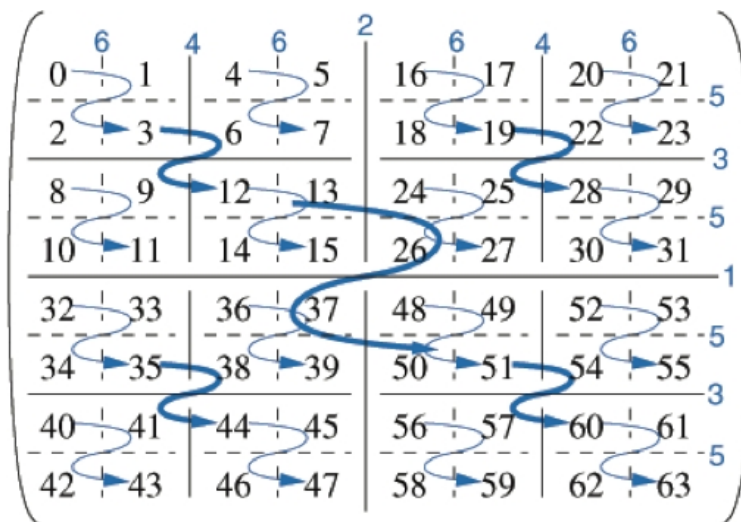
EXTENDED ABSTRACT SUBMITTED FOR PUBLICATION. FOCS99

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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

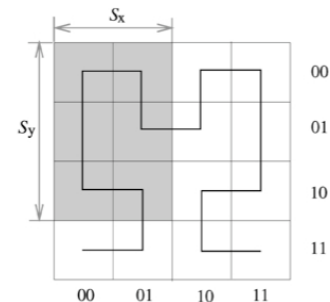
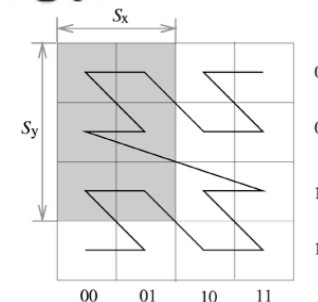
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IEEE TRANSACTIONS ON KNOWLEDGE AND DATA ENGINEERING, VOL. 13, NO. 1, JANUARY/FEBRUARY 2001



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*



Metrics and Models for Reordering Transformations

Morton or Hilbert?

MSP04

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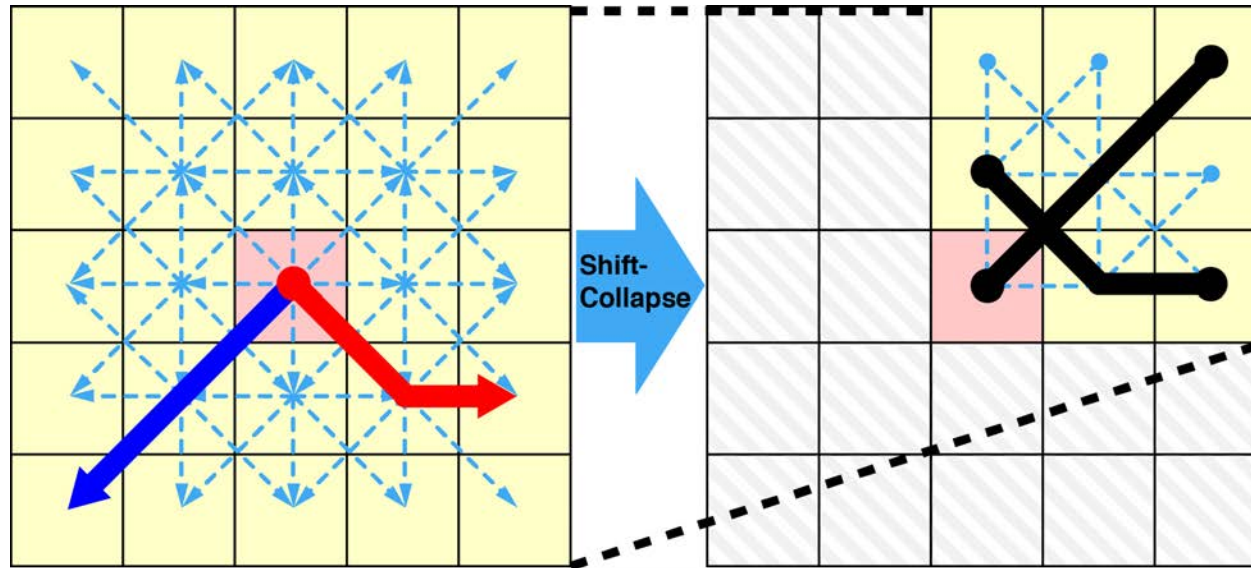
Paul D. Hovland
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Hypergraph

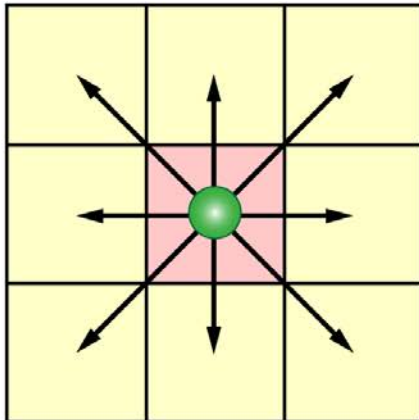
G.M. Morton, "A computer oriented geodetic data base & a new technique in file sequencing,"
IBM Tech. Report ('66)

Shift-Collapse (SC) Algorithm

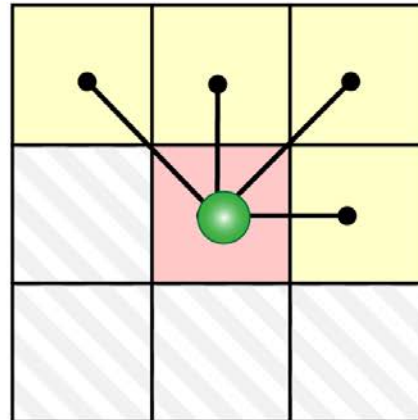
- Generalization of Shaw's eighth-cell method (non-owner-compute method on high-latency cluster) for pair computation to general dynamic range-limited n -tuples



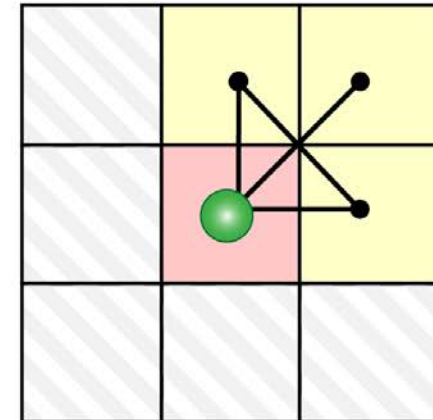
M. Kunaseth *et al.*, *IEEE/ACM Supercomputing (SC13)*



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



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

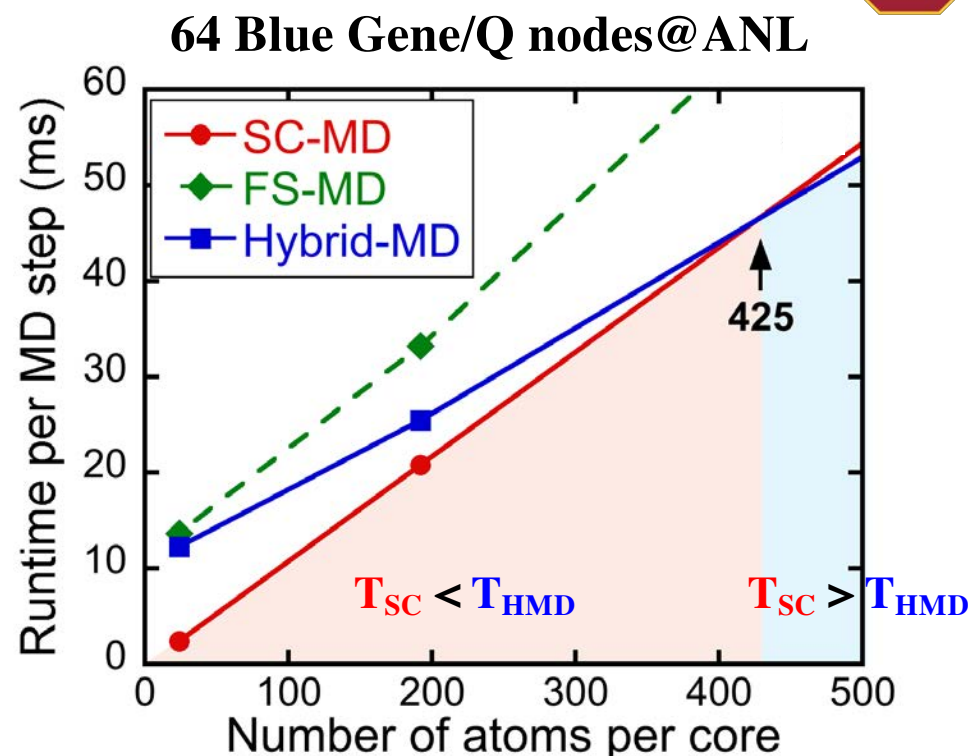
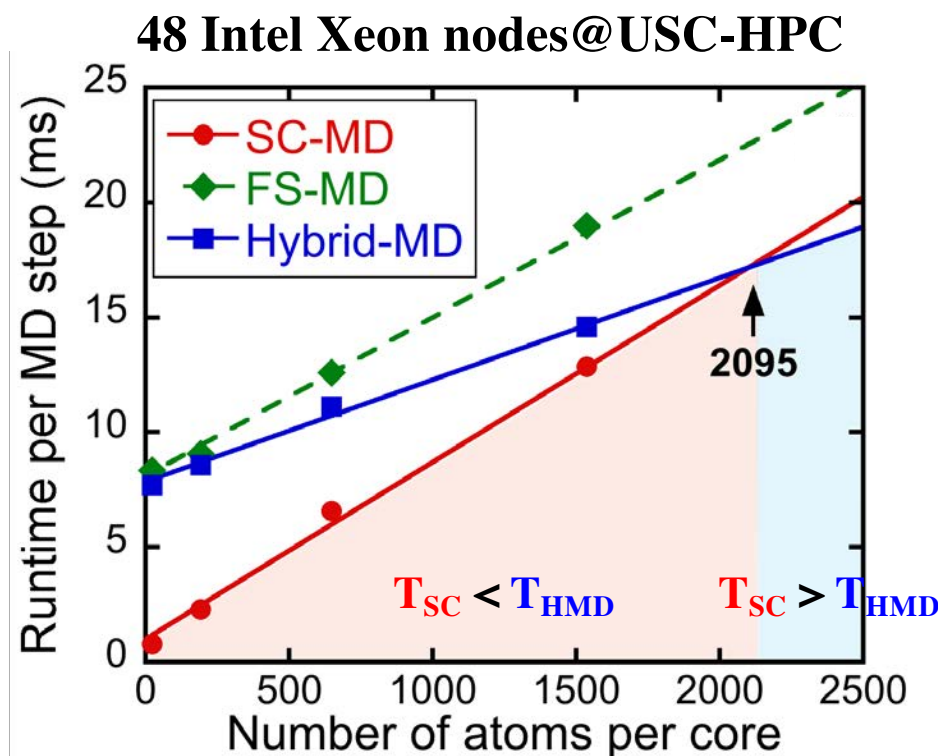


Eighth-shell (ES) method
[Bower *et al.*, '06]

Shift-Collapse (SC) Performance

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

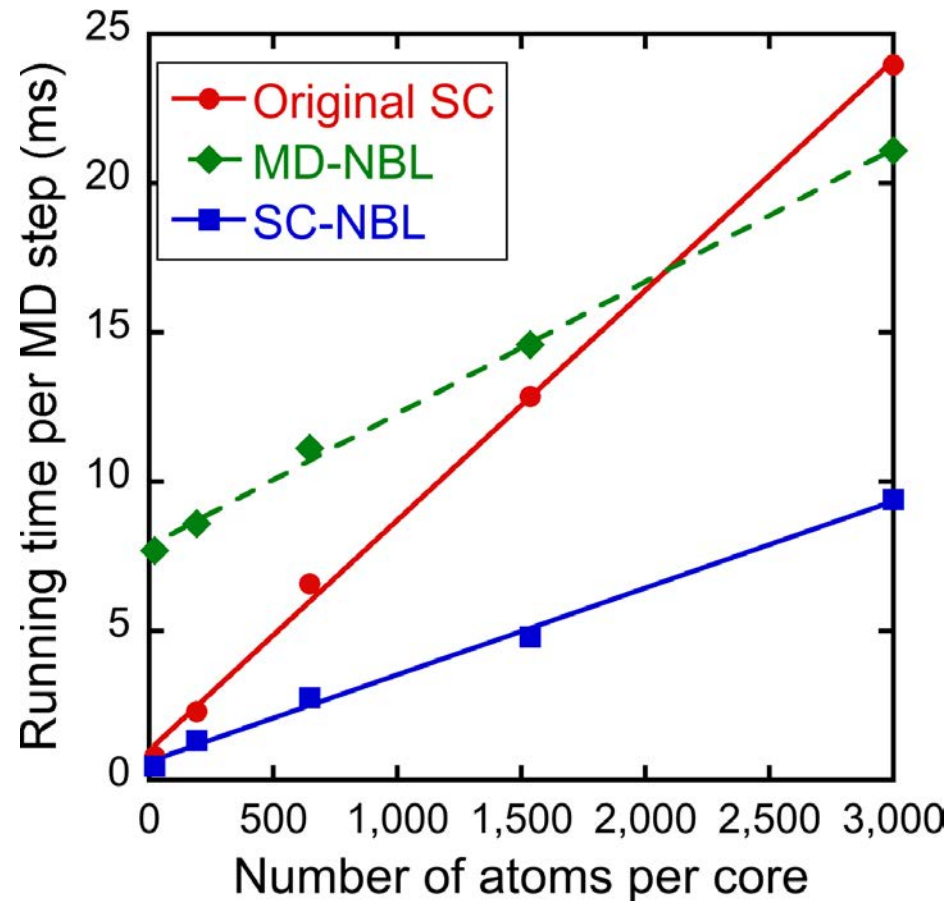
- SC-MD is always faster than FS-MD
- At the smallest grain, SC-MD is **9.7-** and **5.1-fold** speedups over the state-of-the-art hybrid linked-cell & neighbor list code
- Crossover of optimal algorithm from SC-MD to hybrid MD at larger granularity (*i.e.* $N/P > 2,095$ on Intel Xeon and $N/P > 425$)



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)