# Neutral Territory Decomposition for Parallel MD

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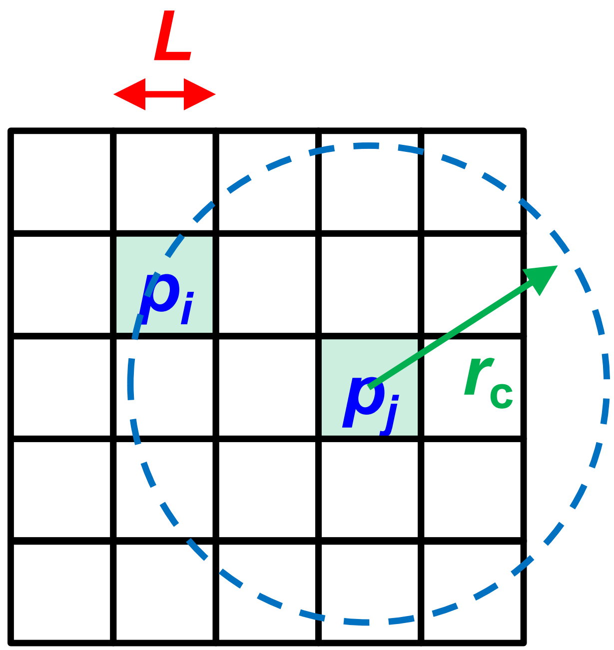
D. E. Shaw, A fast, scalable method for the parallel evaluation of distance-limited pairwise particle interactions, *J. Comput. Chem*. **26**, 1318 ('05)

# Fine Granularity

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

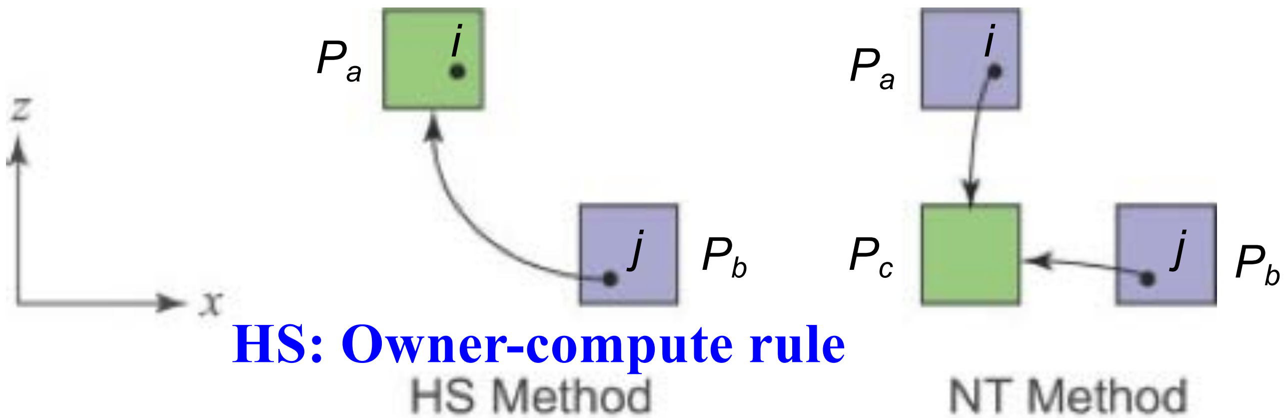
***cf*. Biomolecular simulations**




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

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

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

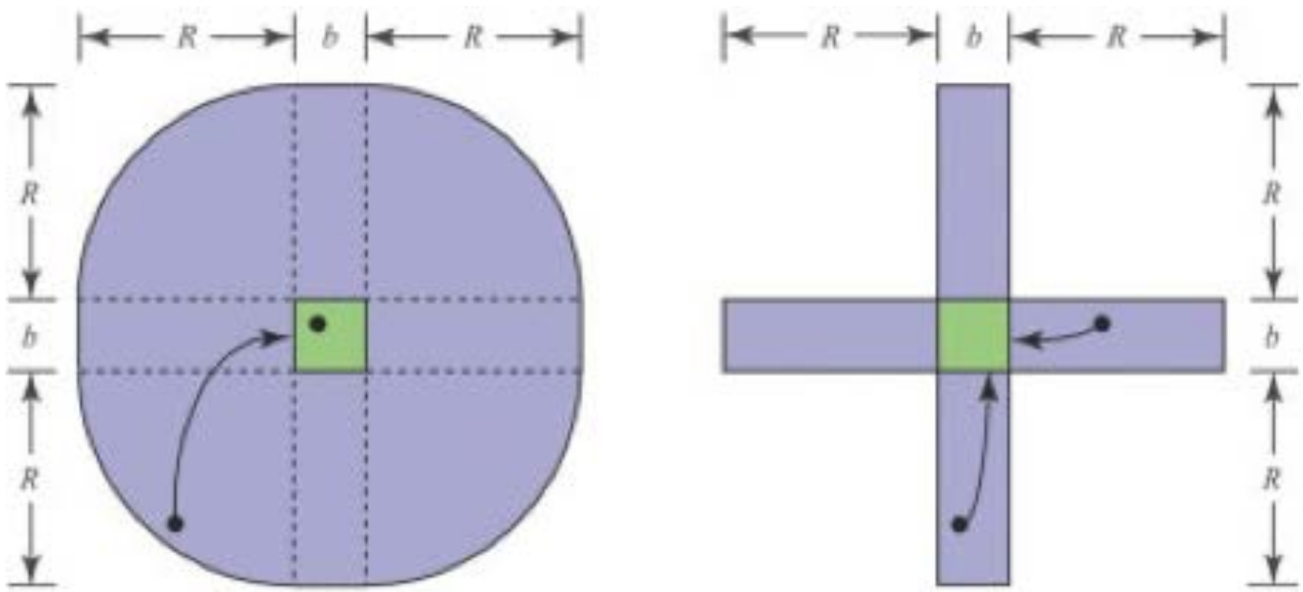



**HS: Owner-compute rule**

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

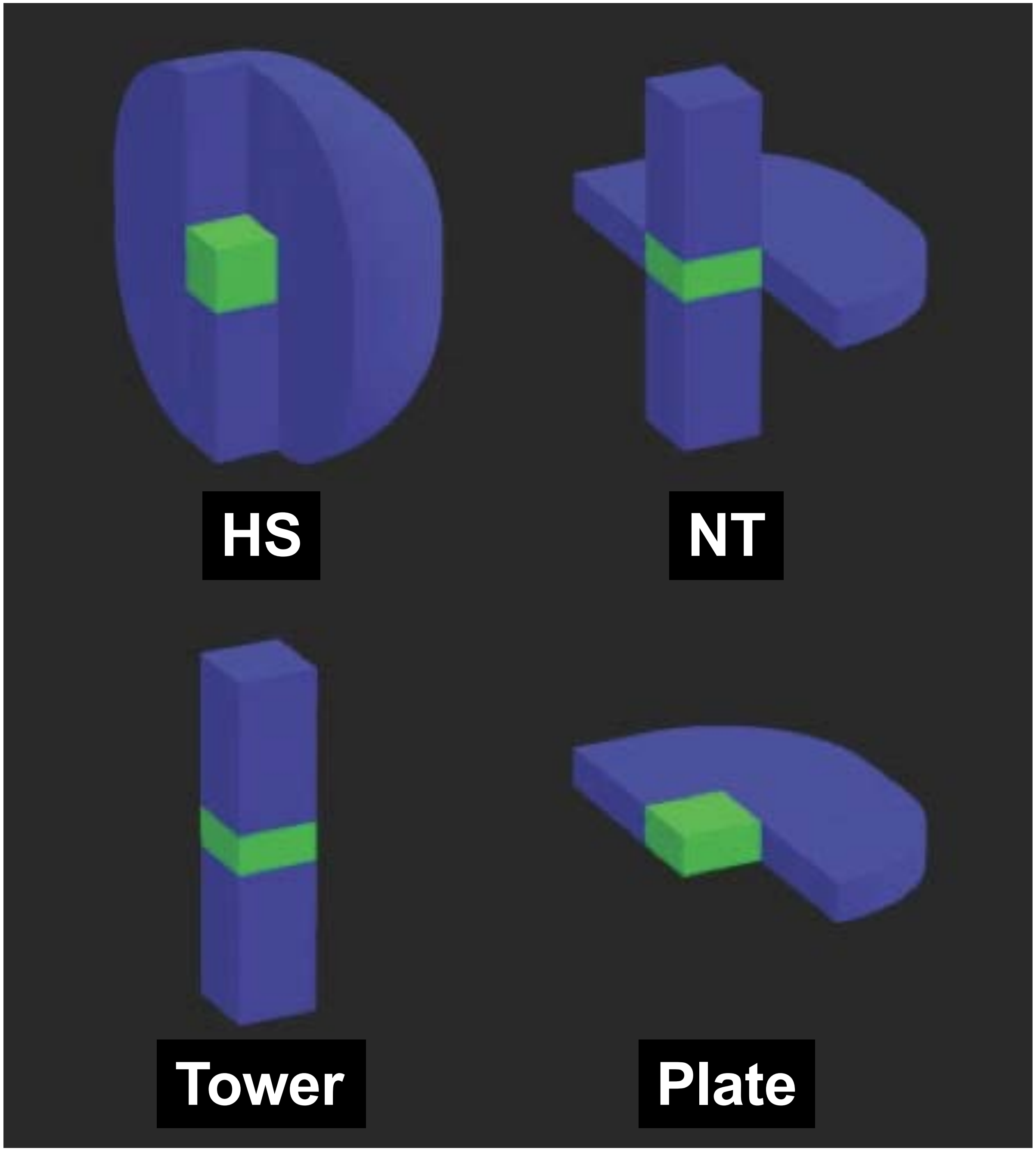
**Import regions or communication volume (2-dimensional example)**

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

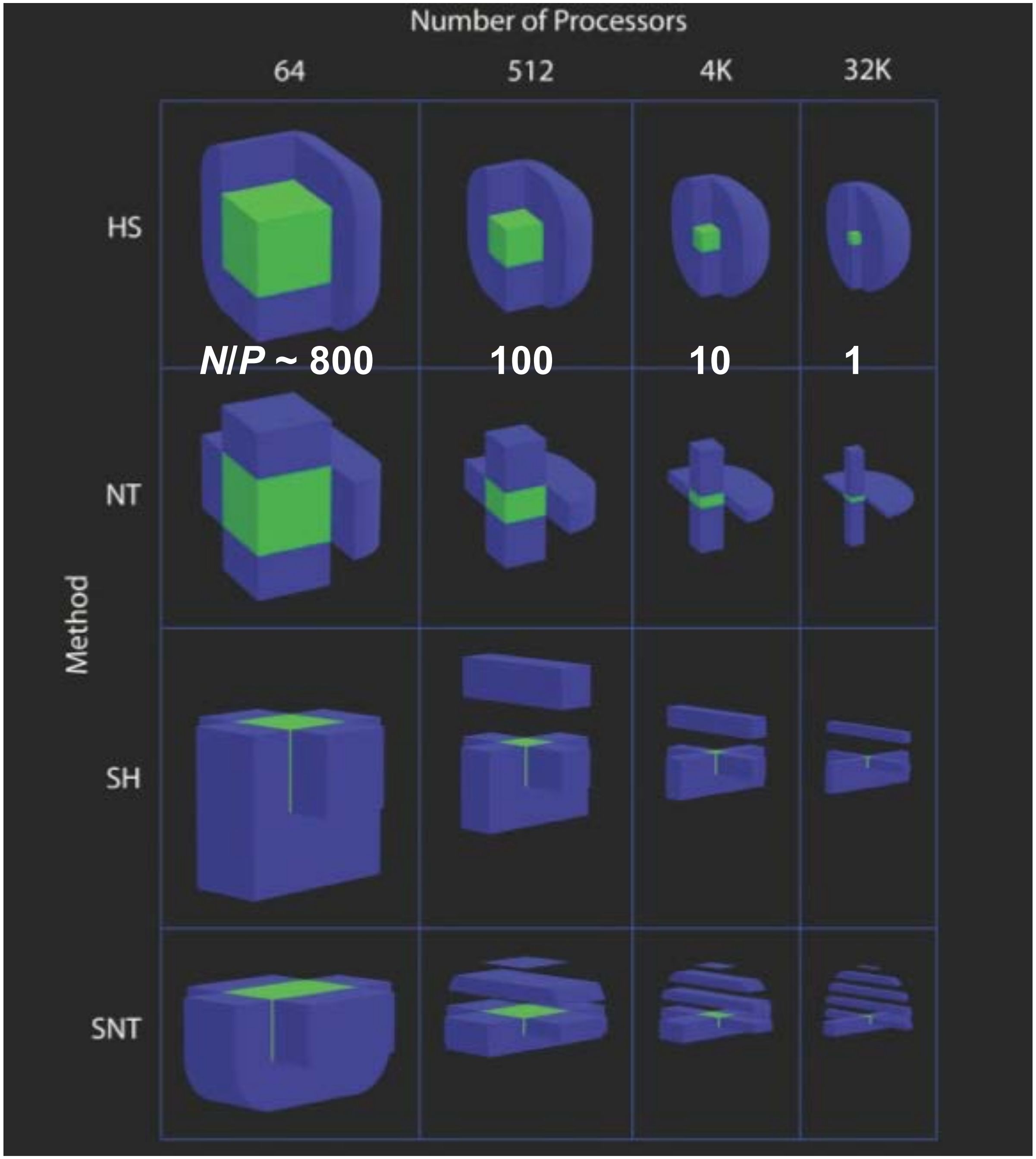



**NT**
**$4bR$**
**$\rightarrow 0$**
**($b\rightarrow 0$)**

# 3D Import Regions



# Scaling of Import Regions




Marc Snir

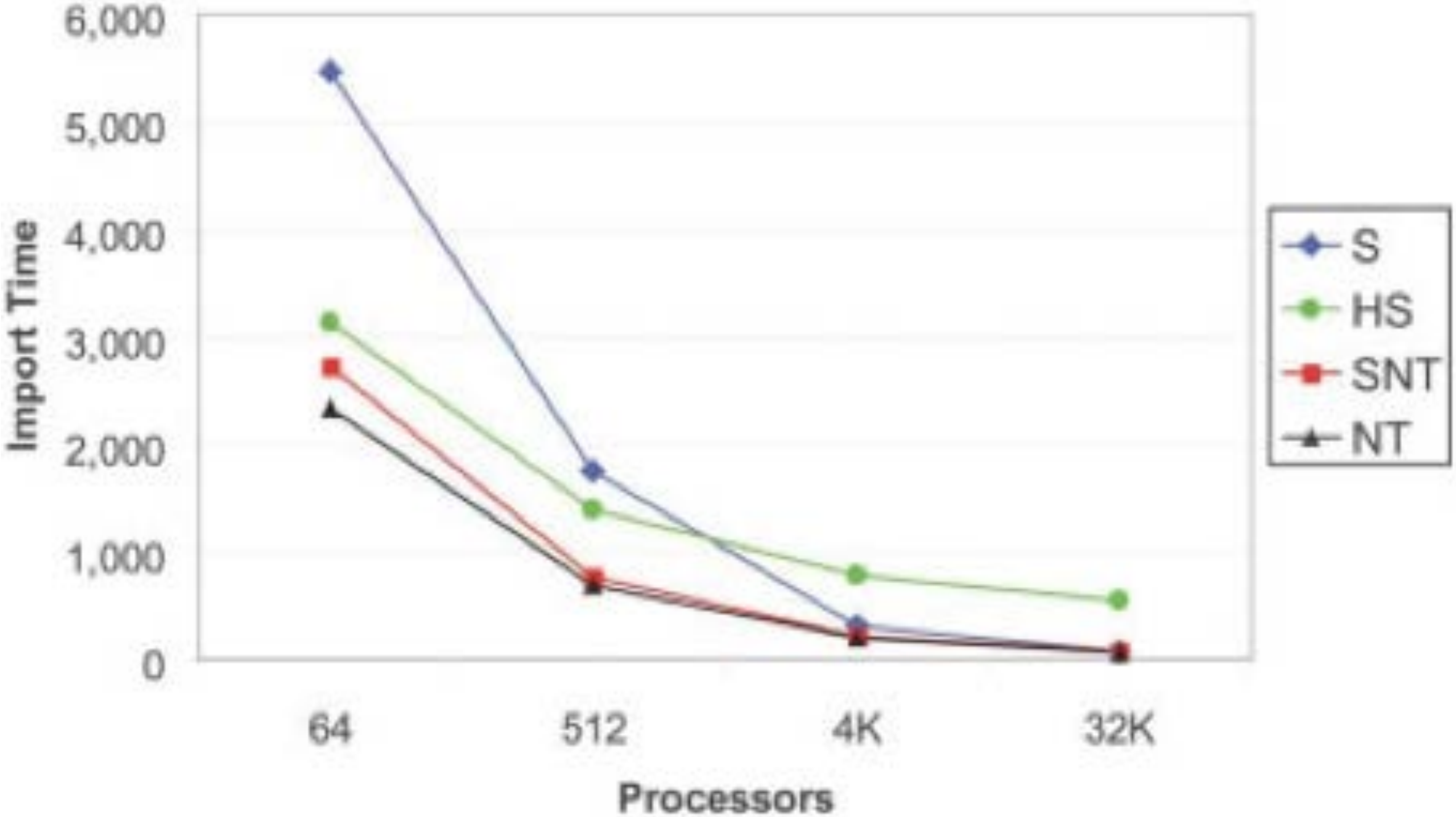
# Scaling of the Volume of Import Regions

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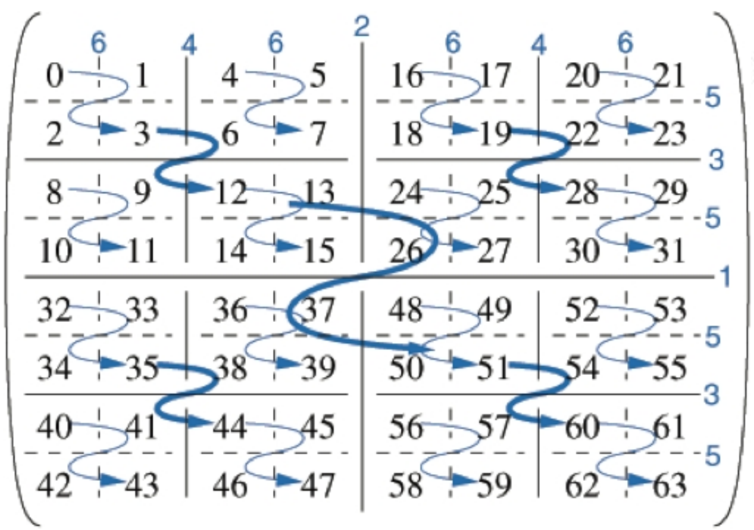
### Recursive Blocked Algorithms and Hybrid Data Structures for Dense Matrix Library Software*

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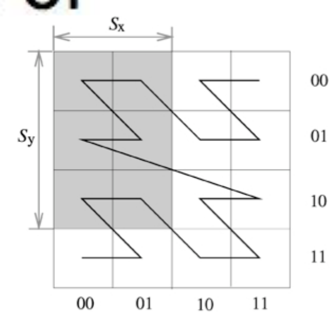
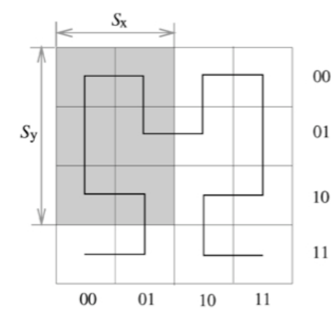
Analysis of the Clustering Properties of the Hilbert Space-Filling Curve


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


**Morton or Hilbert?**

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

**Metrics and Models for Reordering Transformations**

MSP04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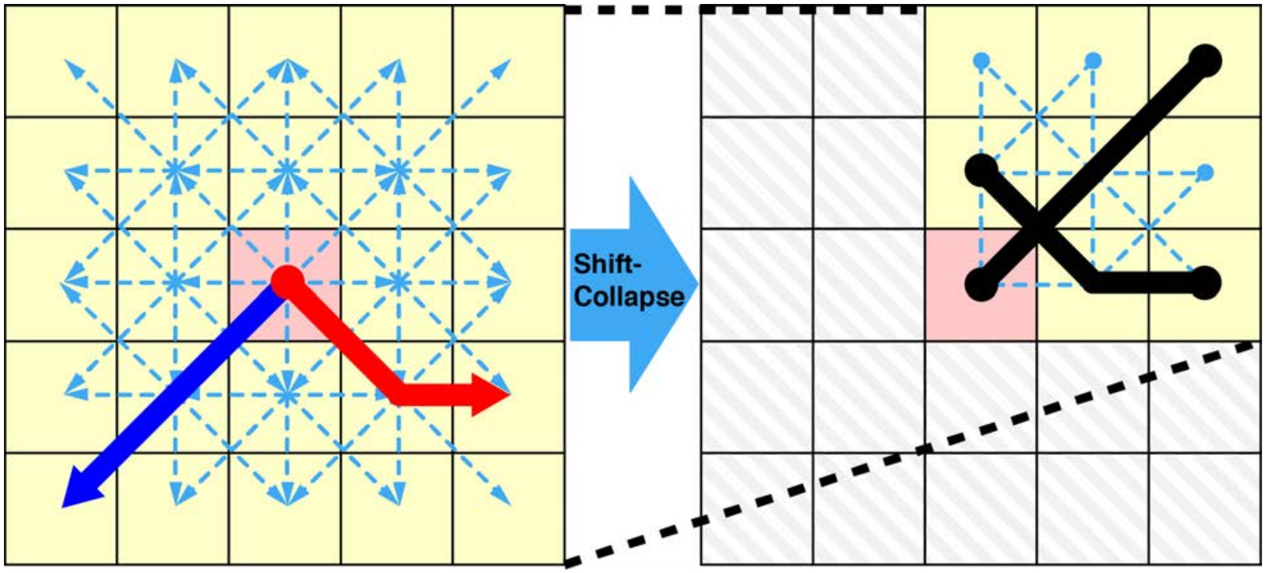
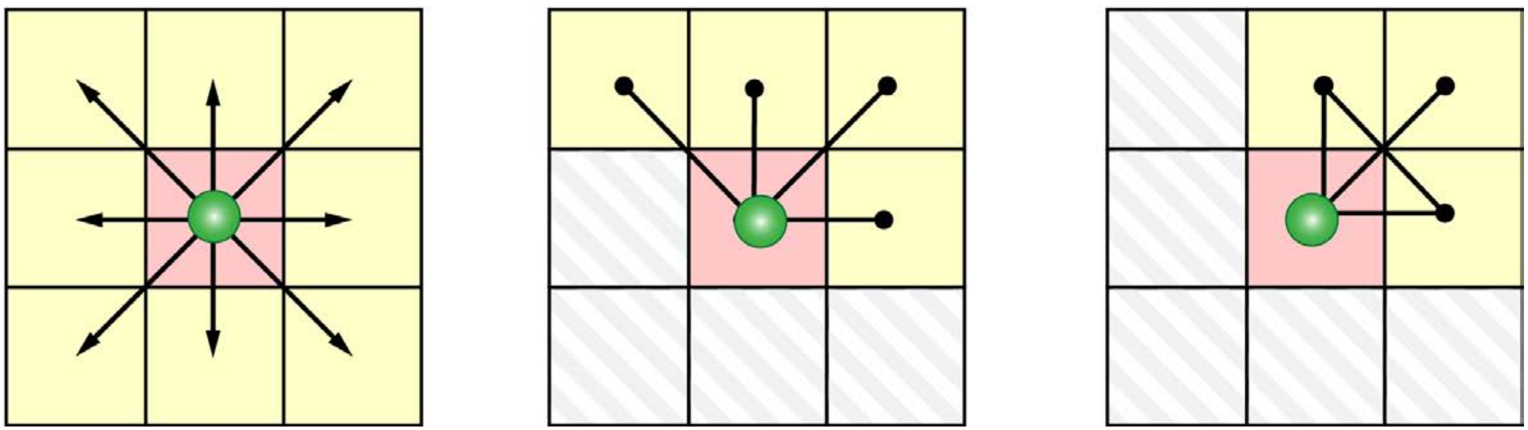
**Hypergraph**

# 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]

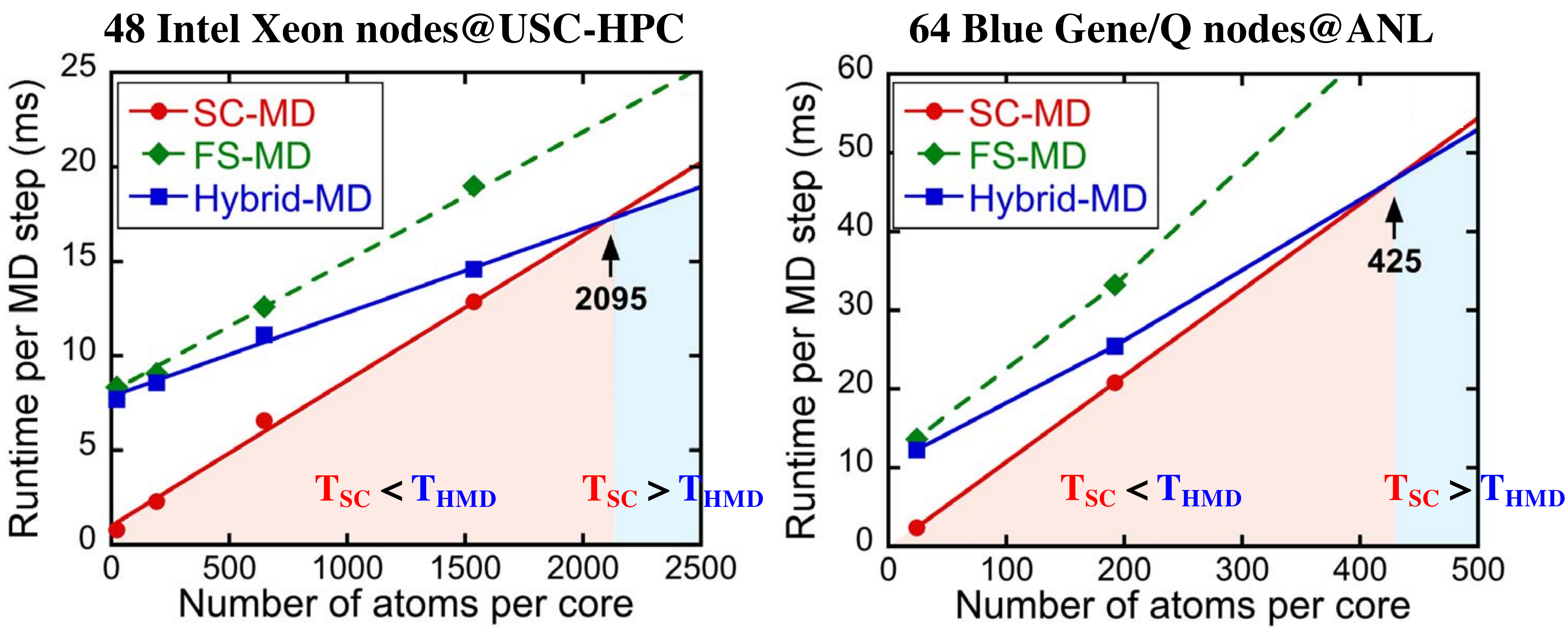
**Half-shell (HS) method**
[*e.g*. Rappaport, '88]

**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**

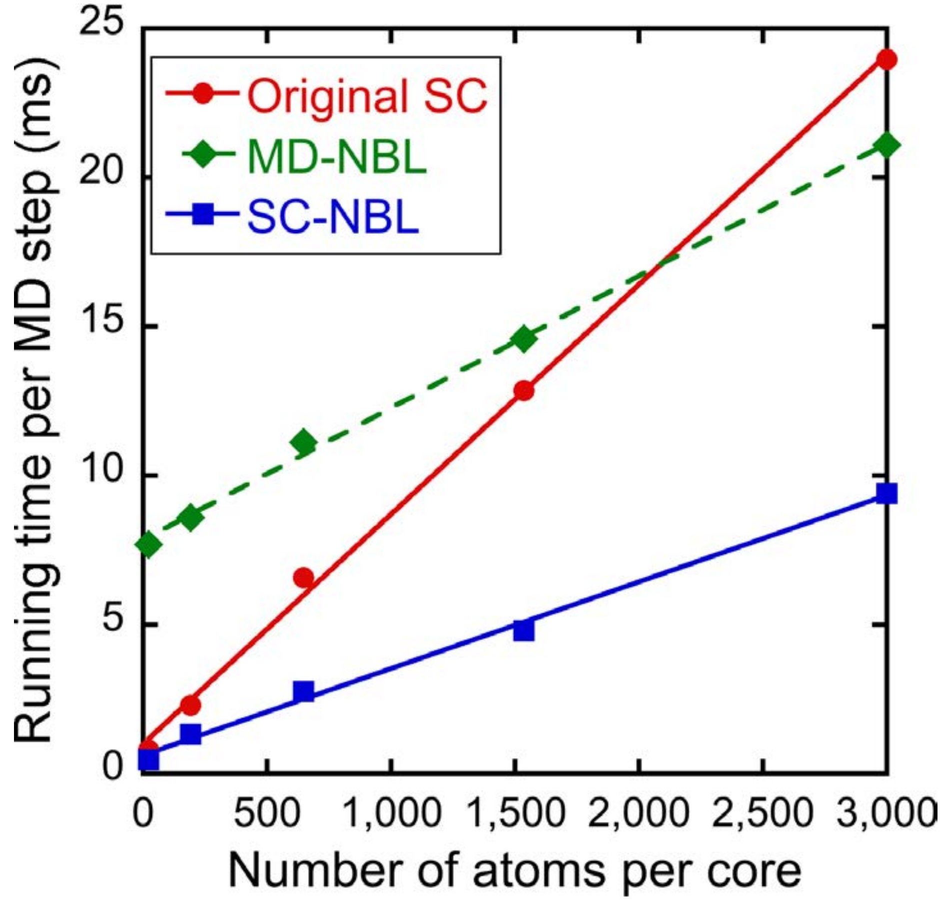
- **SC-MD is always faster than FS-MD**
- **At the smallest grain, SC-MD is 9.7- and 5.1-fold speedups over the state-of-the-art hybrid linked-cell & neighbor list code**
- **Crossover of optimal algorithm from SC-MD to hybrid MD at larger granularity (*i.e.* $N/P > 2{,}095$ on Intel Xeon and $N/P >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




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)**