Neutral Territory Decomposition for Parallel MD

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Fine Granularity

Number of atoms per process ($N/P \sim 1$)

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

HS: Owner-compute rule

Import regions or communication volume (2-dimensional example)

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

NT
\[ 4bR \rightarrow 0 \quad (b \rightarrow 0) \]
3D Import Regions

HS

NT

Tower

Plate
Scaling of Import Regions

\[ \frac{N}{P} \sim 800 \]

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
\[ T_{\text{comm}} = t_{\text{latency}} N_{\text{message}} + \frac{1}{b_{\text{bandwidth}}} V_{\text{message}} \]

# of messages: ns \sim many \mu s

volume (Bytes) of messages
Combine NT with ...

Cache-obliviuous recursive blocking?

Cache-Obliviuous Algorithms
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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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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?

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

Morton or Hilbert?
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)
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)