Neutral Territory Decomposition for Parallel MD

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Spatial (Half-Shell) vs. NT Decompositions

Locus of interaction (2-dimensional example)

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

Import regions or communication volume (2-dimensional example)

HS

\[ 4bR + \pi R^2 \xrightarrow{b \to 0} \text{const.} \]

NT

\[ 4bR \xrightarrow{b \to 0} 0 \]
3D Import Regions

HS
NT
Tower
Plate
### Scaling of Import Regions

**Equation:**

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

**Methods:**
- HS
- NT
- SH
- SNT

**Number of Processors:**
- 64
- 512
- 4K
- 32K

**Values:**
- HS: 100, 10, 1
- NT: 100, 10, 1
- SH: 10, 1
- SNT: 10, 1

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

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

\( ns \sim \text{many } \mu s \)
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†
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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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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?

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

Hypergraph
Reactive Molecular Dynamics (RMD)

- Dynamic $n$-tuple computation: $n \leq 4$ explicitly; $\leq 6$ through bond order

$$f_i^{(n)} = - \sum_{\forall (r_0, ..., r_{n-1}) \in \Gamma^{(n)}} \frac{\partial}{\partial x_i} \Phi_n(x_0, ..., x_{n-1}) \bigg|_{(x_0, ..., x_{n-1})=(r_0, ..., r_{n-1})}$$

(a) $n=2$  (b) $n=3$  (c) $n=4$

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 and 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)