Neutral Territory Decomposition for Parallel MD

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California

Email: anakano@usc.edu

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-computes 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**

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

\[ \text{ns} \sim \text{many } \mu\text{s} \]

\[ \text{volume (Bytes) of messages} \]
Combine NT with ...

Cache-oblivious recursive blocking?

Cache-Oblivious Algorithms
EXTENDED ABSTRACT SUBMITTED FOR PUBLICATION. FOCS99

Matteo Frigo Charles E. Leiserson Harald Prokop Sridhar Ramachandran
MIT Laboratory for Computer Science, 545 Technology Square, Cambridge, MA 02139
{athena, cel, prokop, sridhar}@supertech.lcs.mit.edu

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*

John Mellor-Crummey†, David Whalley‡, Ken Kennedy†

† Department of Computer Science, MS 132
Rice University
6100 Main
Houston, TX 77005
{johnmc,ken}@cs.rice.edu

‡ Computer Science Department
Florida State University
Tallahassee, FL 32306-4530
whalley@cs.fsu.edu
phone: (850) 644-3506

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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

Michelle Mills Strout
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, IL 60439 USA
mstrout@mcs.anl.gov

Paul D. Hovland
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, IL 60439 USA
hovland@mcs.anl.gov

ISC99

Morton or Hilbert?

MSP04

Hypergraph

G.M. Morton, “A computer oriented geodetic data base & a new technique in file sequencing,”
IBM Tech. Report ('66)
**Reactive Molecular Dynamics (RMD)**

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

\[
f_i^{(n)} = - \sum_{\forall (r_0, \ldots, r_{n-1}) \in \Gamma^{(n)}} \frac{\partial}{\partial \mathbf{x}_i} \Phi_n (\mathbf{x}_0, \ldots, \mathbf{x}_{n-1}) \bigg|_{(\mathbf{x}_0, \ldots, \mathbf{x}_{n-1})=(r_0, \ldots, r_{n-1})}
\]

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

K. Nomura et al.,  
*Comp. Phys. Commun.* **192**, 91 ('15)
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)