XLBIOSIM

Molecular Modeling Acceleration Systems

Reconfigurable hardware molecular dynamics acceleration on Cray XD1: the system approach

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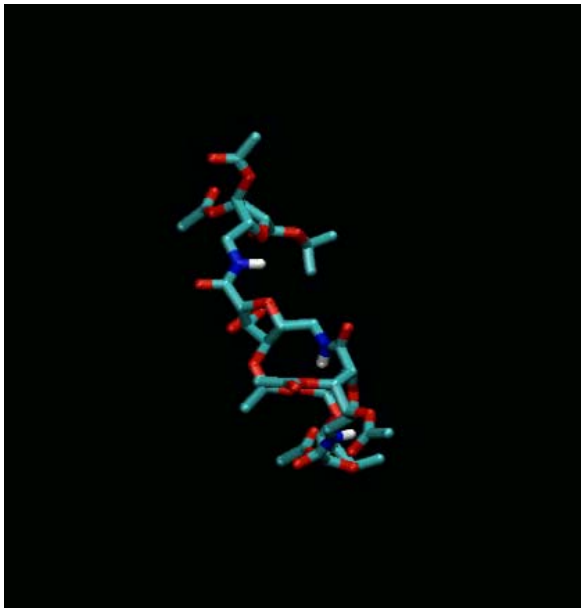
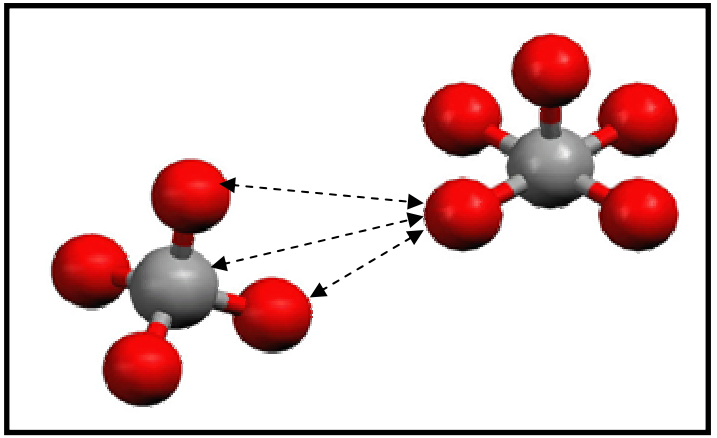
MD for bio-molecular research

Insightful but slow

100ns 10 weeks





non-bonded interactions:
Coulombic, Lennard-Jones

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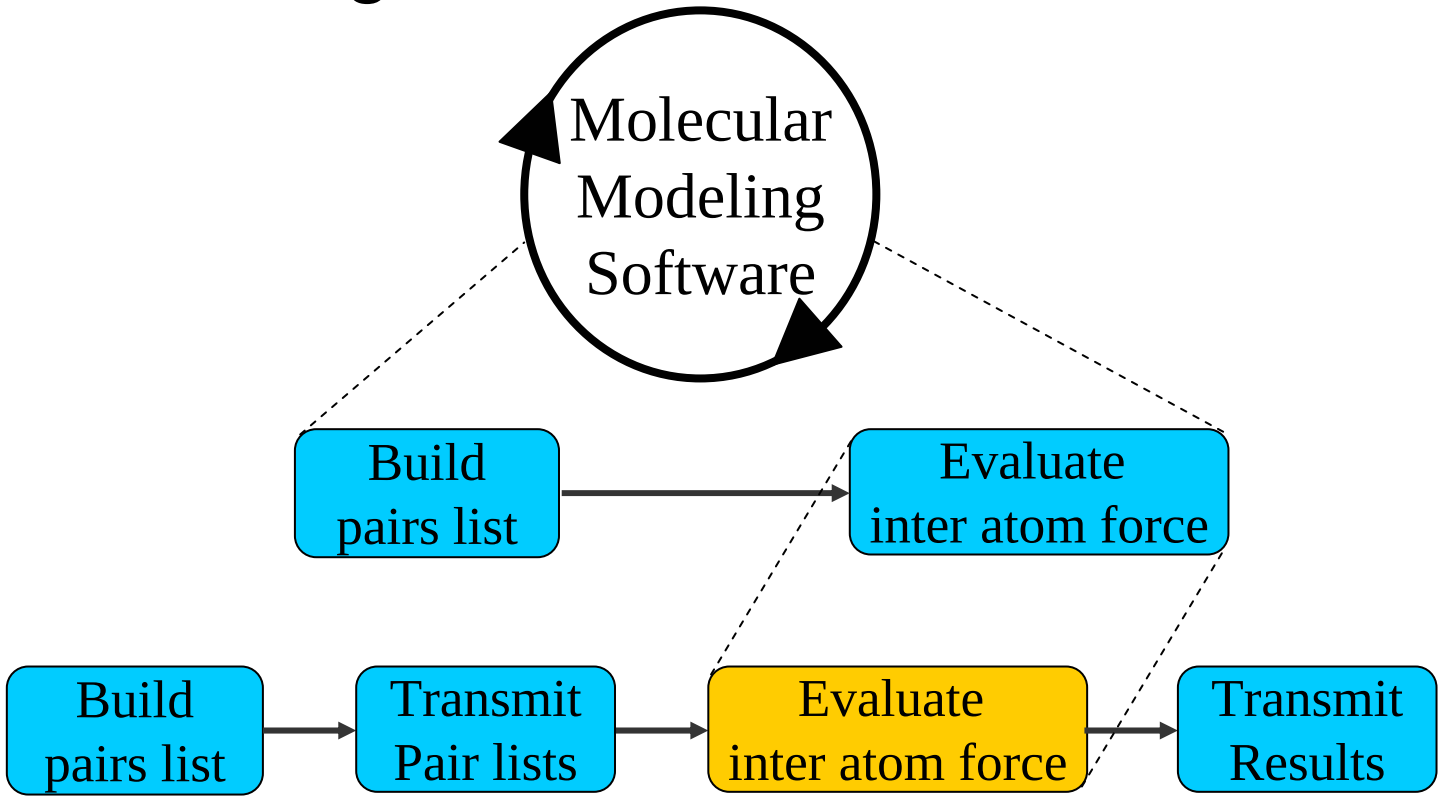
Sequential process

Accelerating the non bonded interactions



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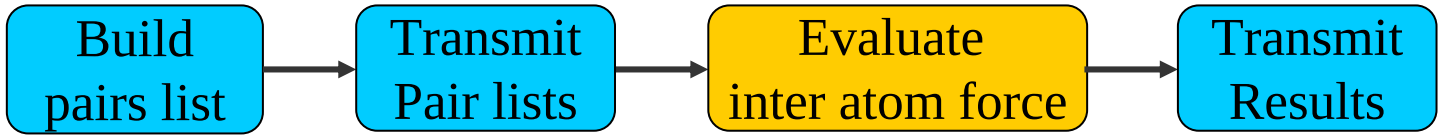
Performance Model

Computation and communication procedures



$$T = t(Ppairs) + t(Cac) + t(Pnbforce) + t(Cproc)$$

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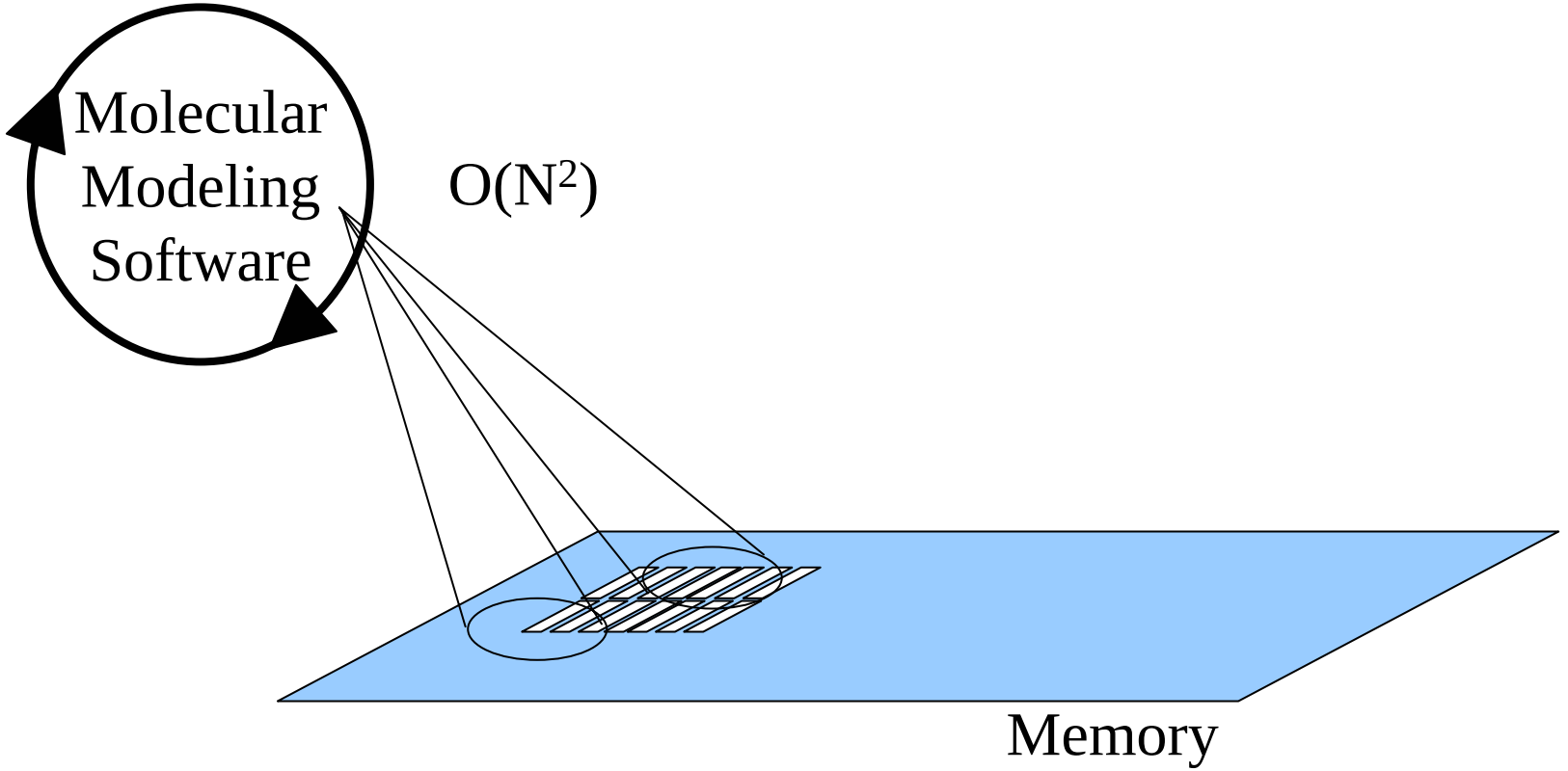
Most SW use exhaustive search

Searching atoms pairs d2 < Rc



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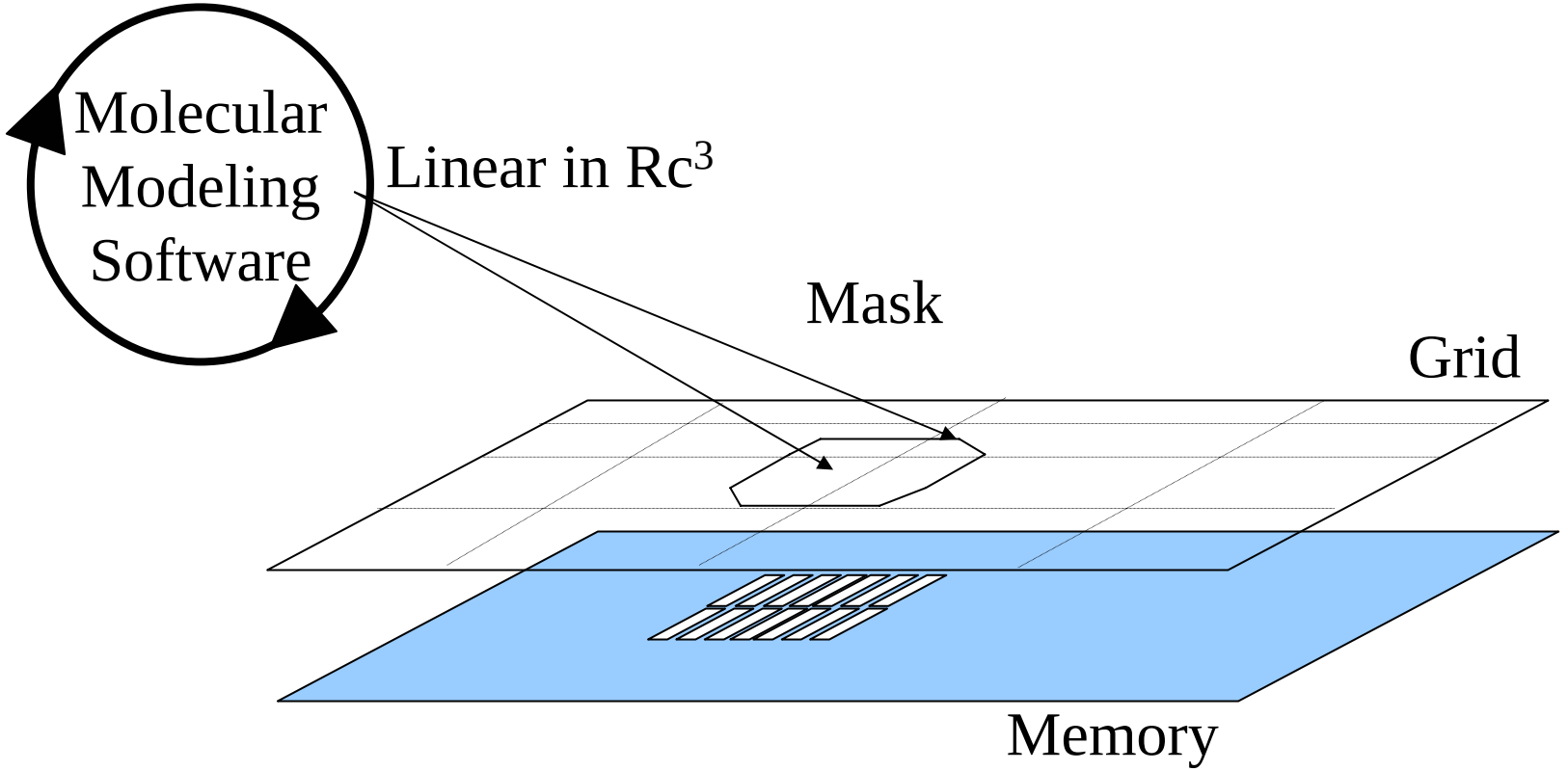
Newer SW use grid Search

Searching atoms pairs d2 < Rc



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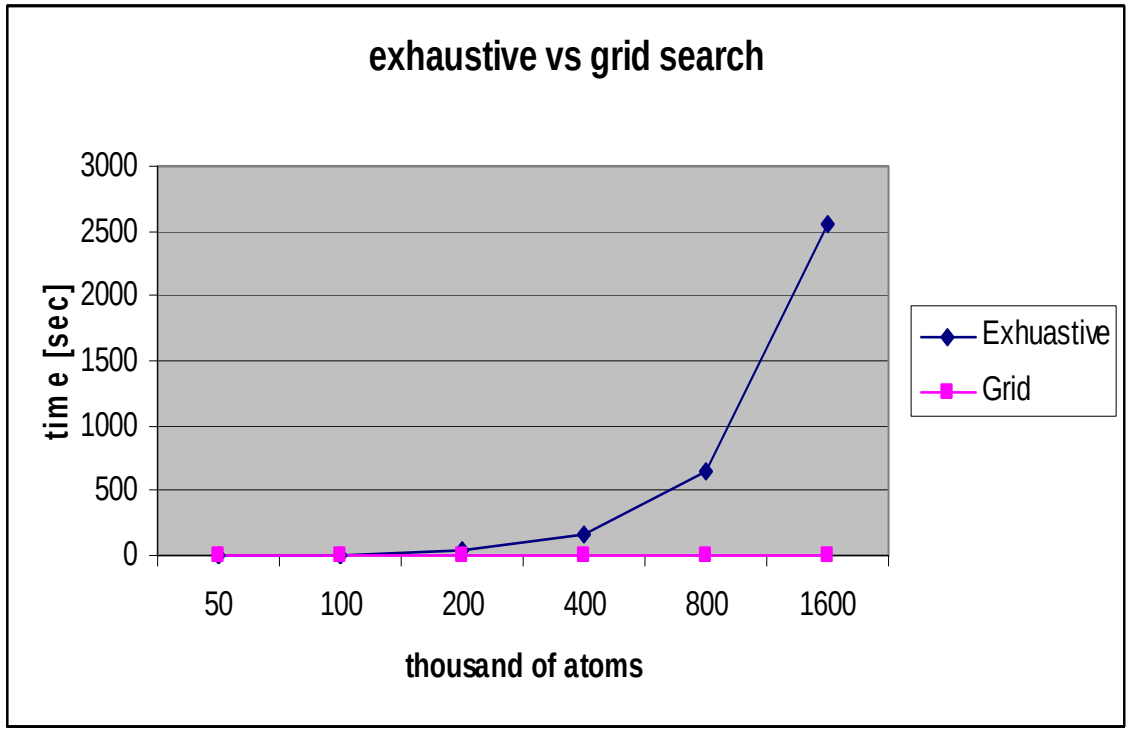
Grid search better for large configurations



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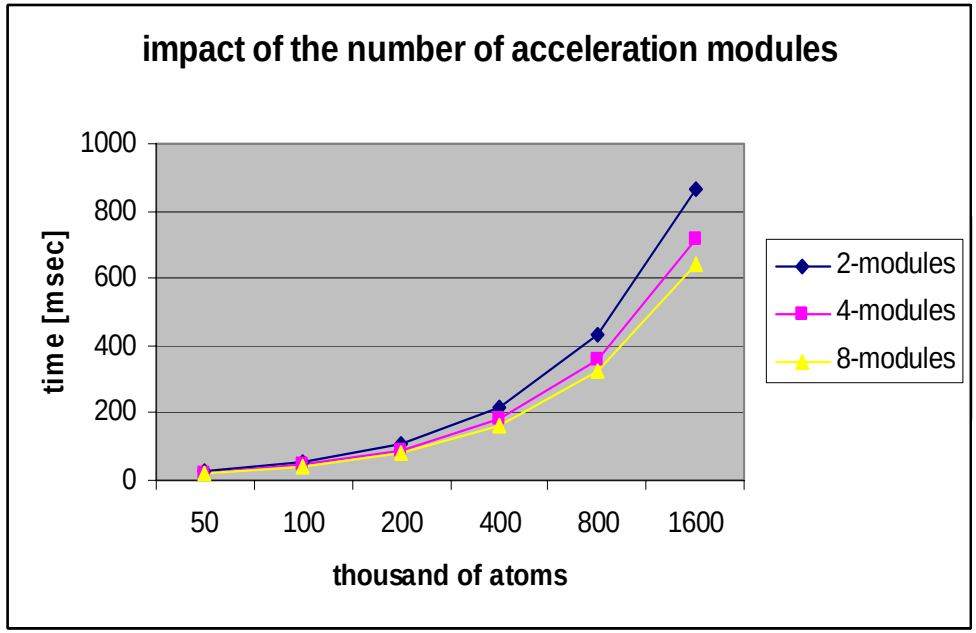
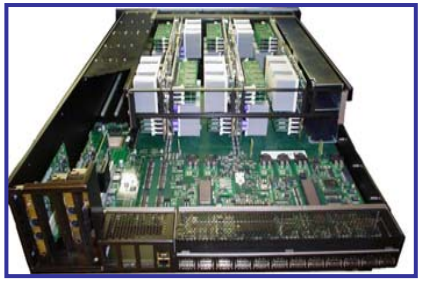
Co-processor speed
not always the performance limit





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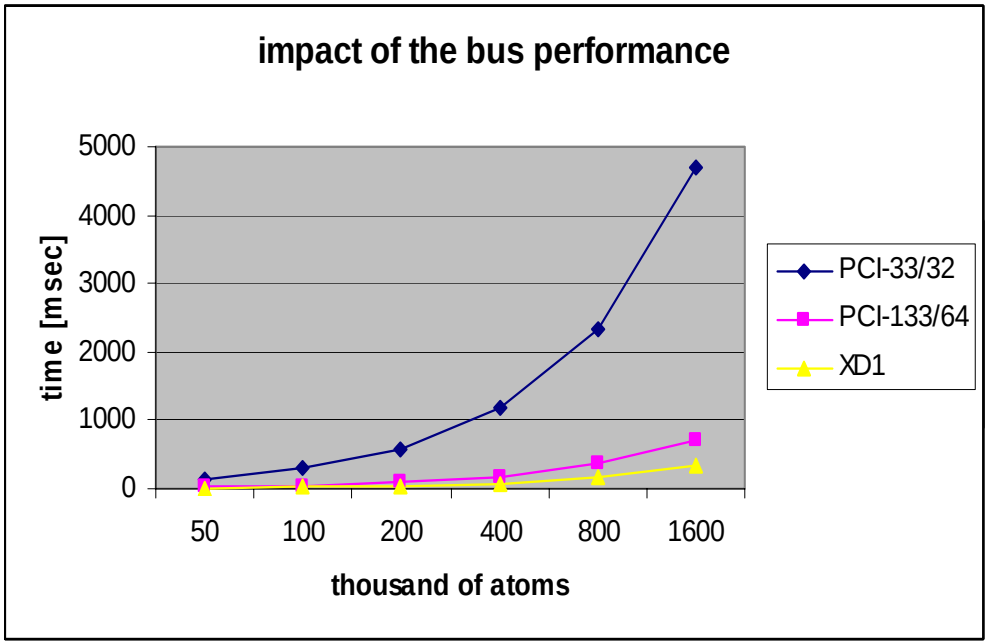
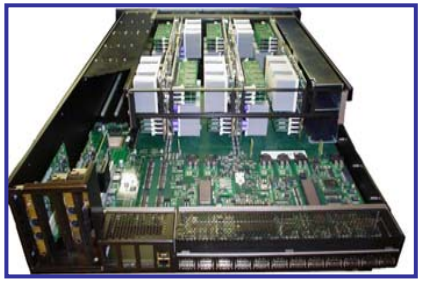
Bus bandwidth

Chip to chip communication is key





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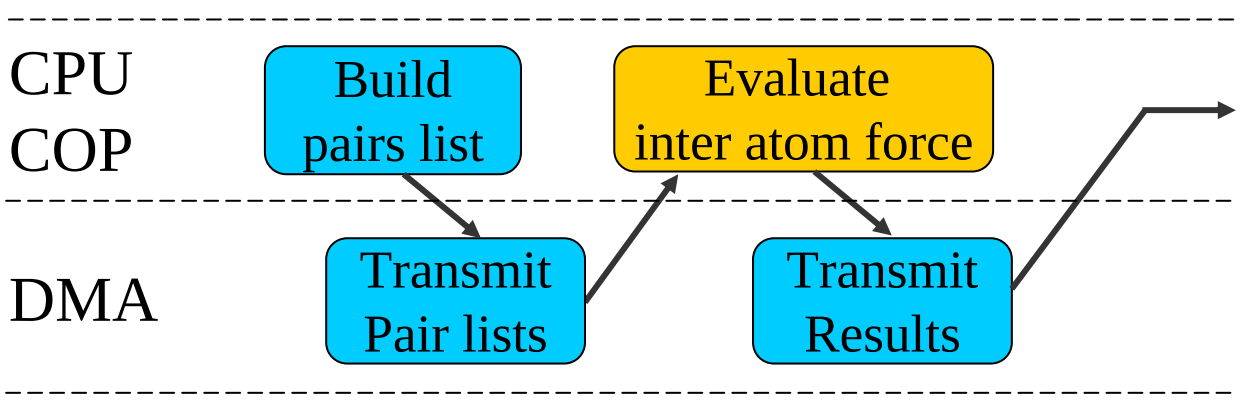
Design efforts on communication

impact on performance similar to better hardware

Data compression

Latency hiding

Larger bus bandwidth



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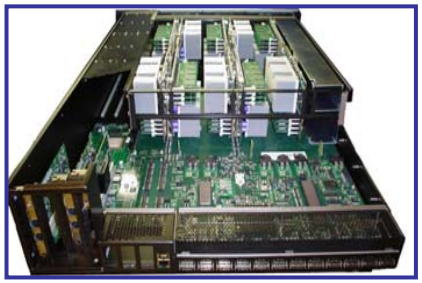
Scalable solution

XLBiosim on XD1

Grid Search+XLB
Fast co-processor

→

CPU to COP
Bus Bandwidth



Gromos MPI+XLB
Parralel implementation

→

CPU to CPU Bandwidth
CPU to COP Bandwidth

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Discussion

Questions / Suggestions ?

Thank you for your attention!

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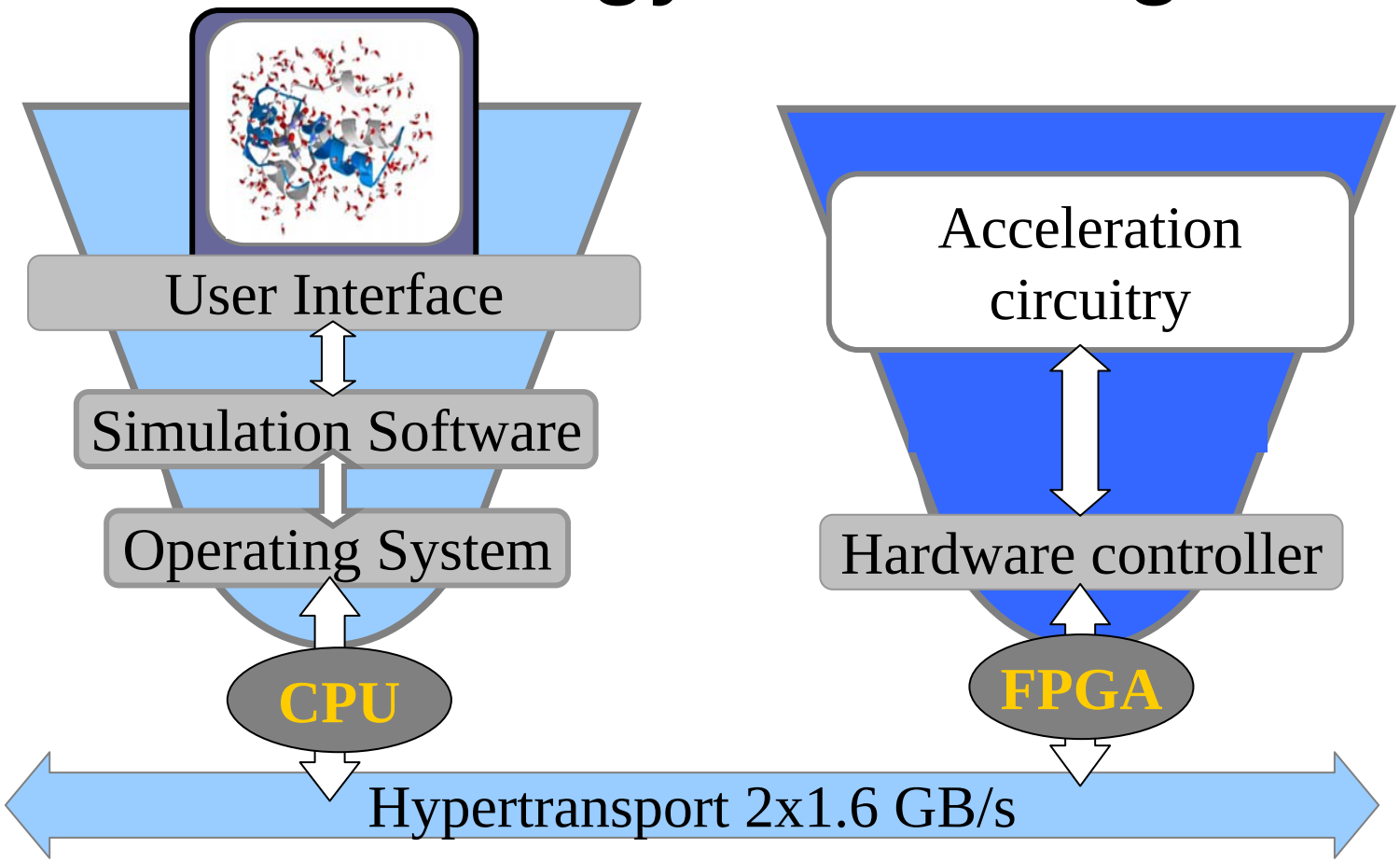
Technology advantage



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Assumptions

Number of atoms	Average number of interacting pairs	Average pair list size
90,000	1,500,000	75

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Assumptions (cont'd)

Constant	Value
cforceCOP (XLBiosim accelerator*)	2
Cmem	24
Rc (nm)	1
Cpairs	2
cres	0.16