FCCM 2004

Reconfigurable Molecular Dynamics Simulator

Navid Azizi, Ian Kuon, Aaron Egier, Ahmad Darabiha and Paul Chow
University of Toronto

Why is Molecular Dynamics interesting?

- Simulates interaction of atoms over time
- Many possible applications
  - Biomolecules
- Computationally intensive to handle >1000 atoms
- Large computer clusters used in the past
- Can a reconfigurable simulation system do this better?

What is Molecular Dynamics?

- Simulate using classical Newtonian mechanics

$$F = m\,a$$

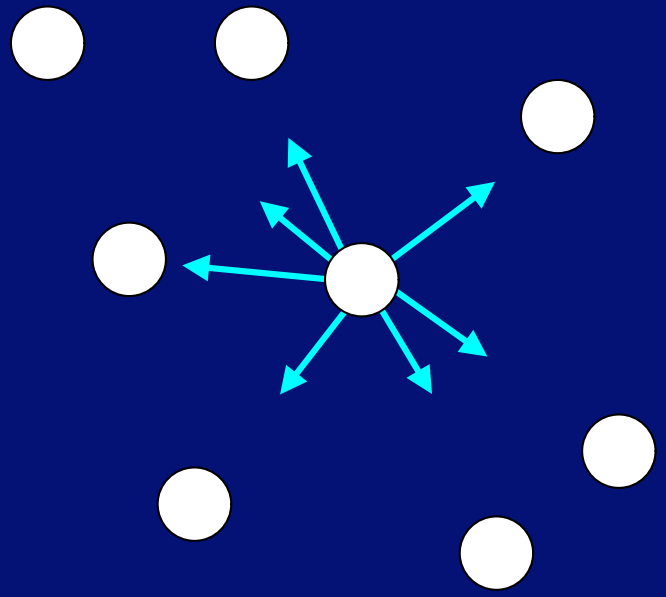
- Integrate acceleration to get position and velocity changes
- Use a very small timestep ~ 1 femtosecond

Molecular Dynamics Background

- Simulation Procedure per timestep
  - Sum force over all interacting atoms
  - Calculate acceleration
  - Integrate acceleration to update atom position and velocity
  - Repeat for all atoms

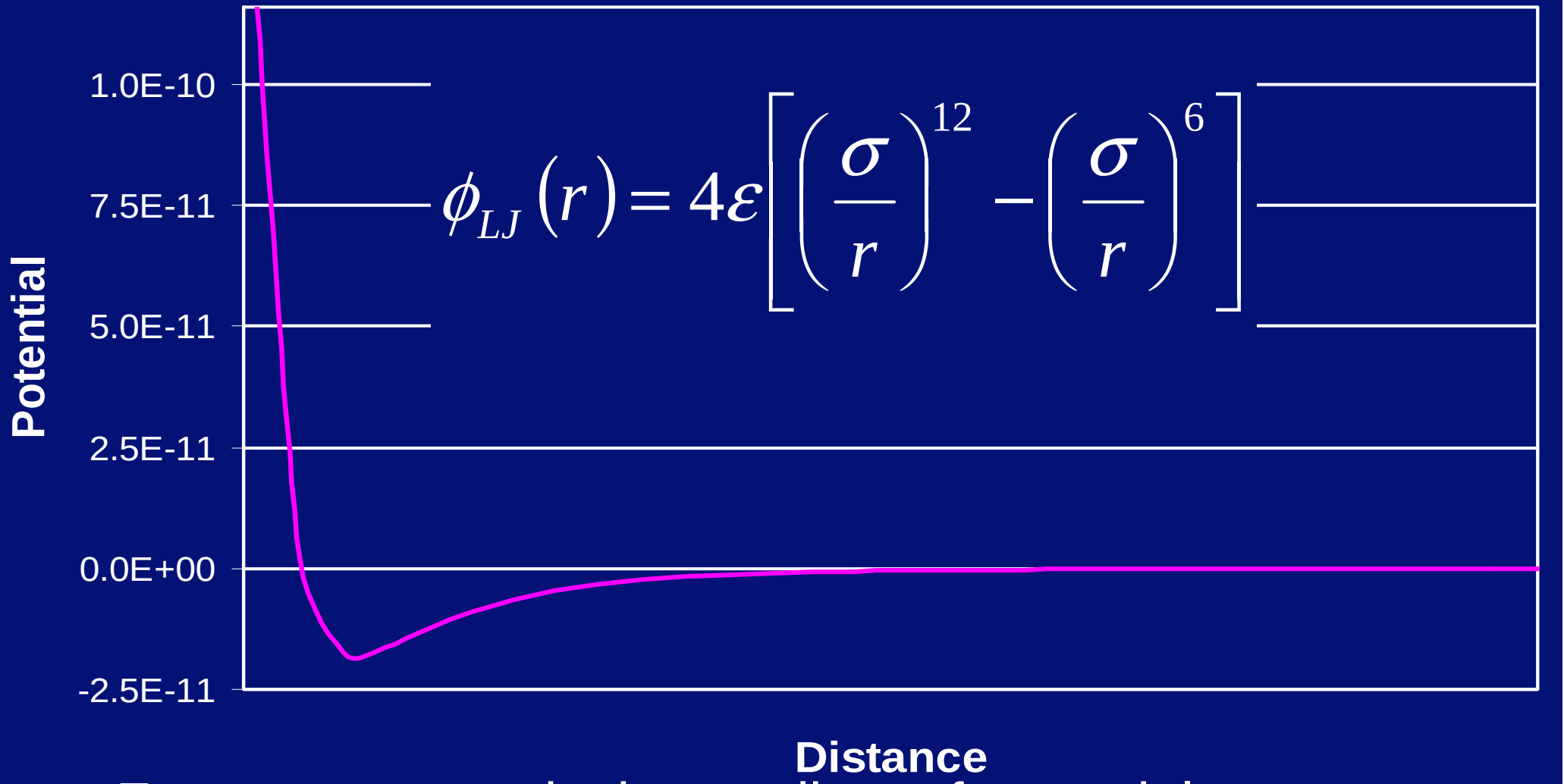
Background - Forces

- Two types of forces
  - –Bonded – O(n)
    - –No hardware acceleration required
  - –Non Bonded – $O(n^2)$
    - –Needs hardware acceleration



Background – Force Calculation

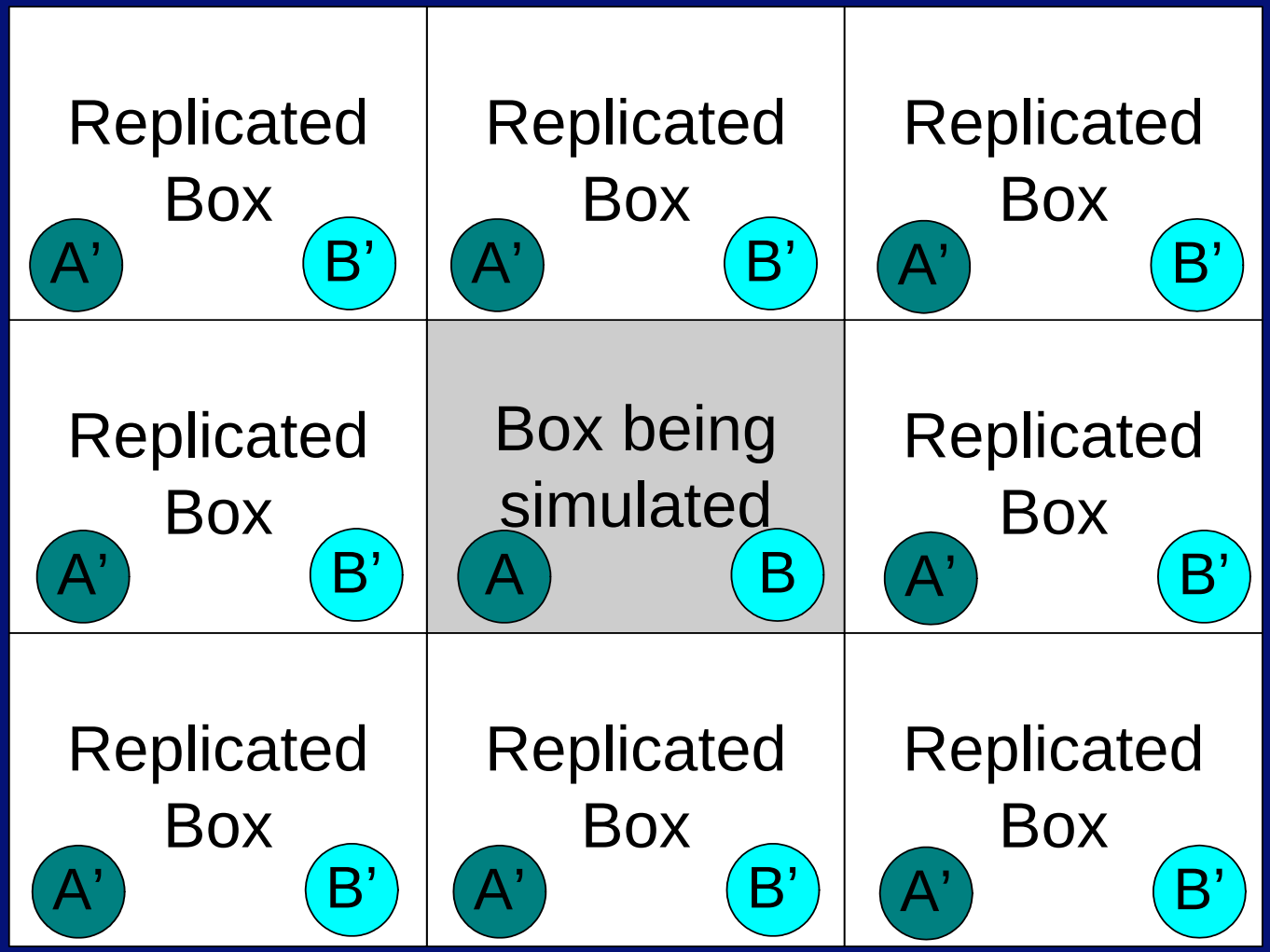
- Lennard-Jones (LJ) potential models interaction



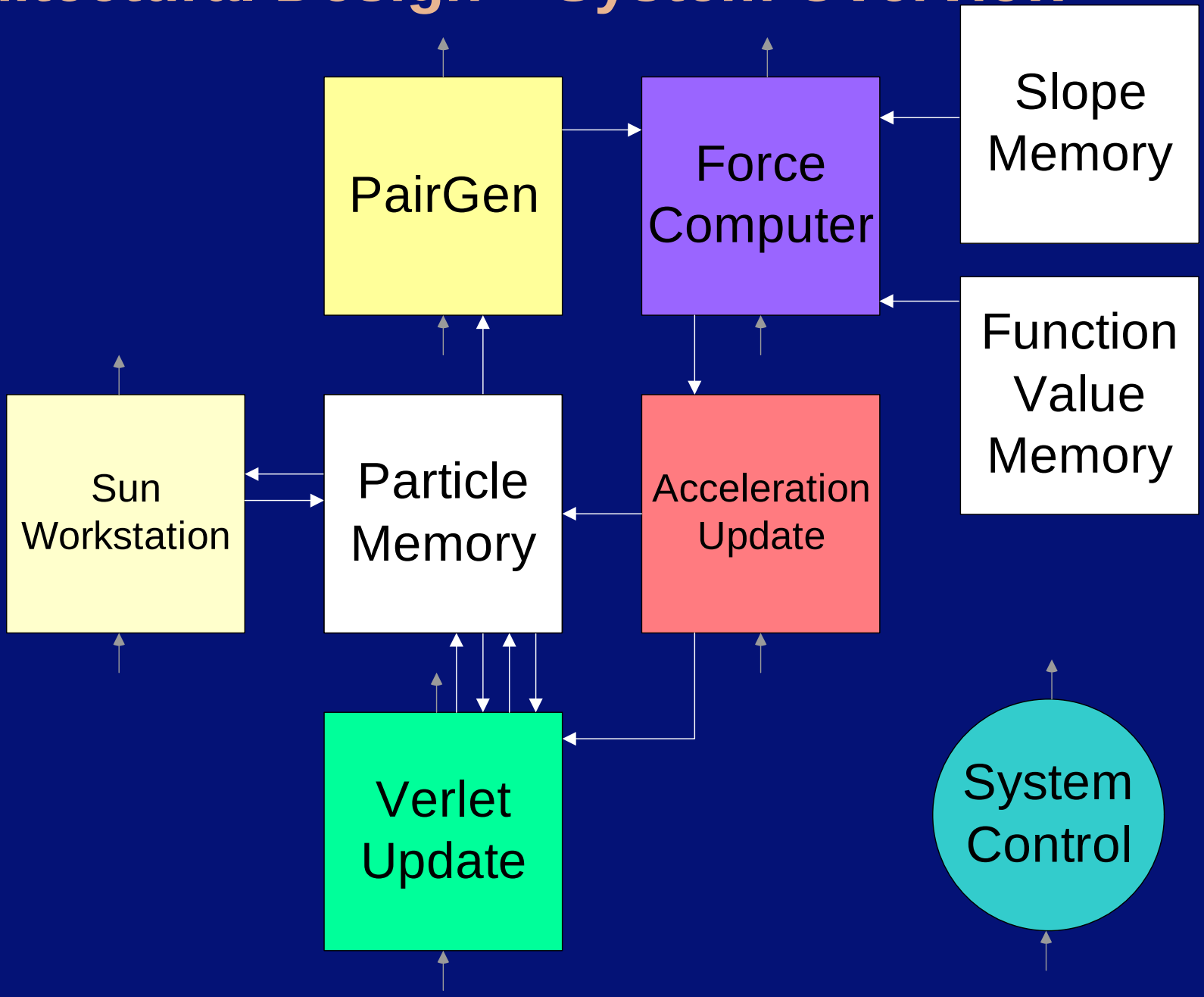
- Force on a atom is the gradient of potential

Background – Simulating Large Volumes

- Any interesting volume has far too many atoms to simulate
- Solution – Periodic Boundary Conditions

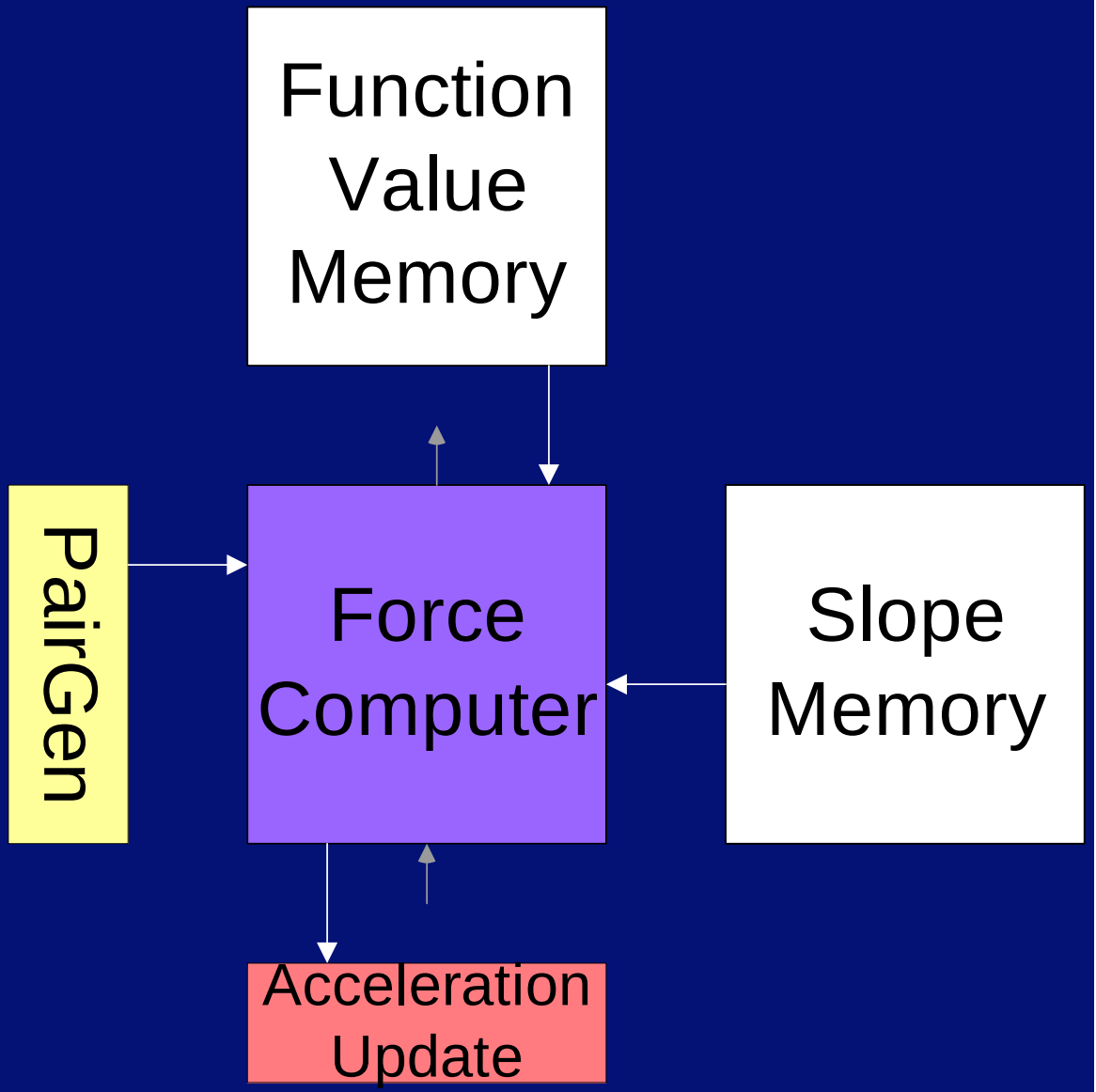


Architectural Design – System Overview



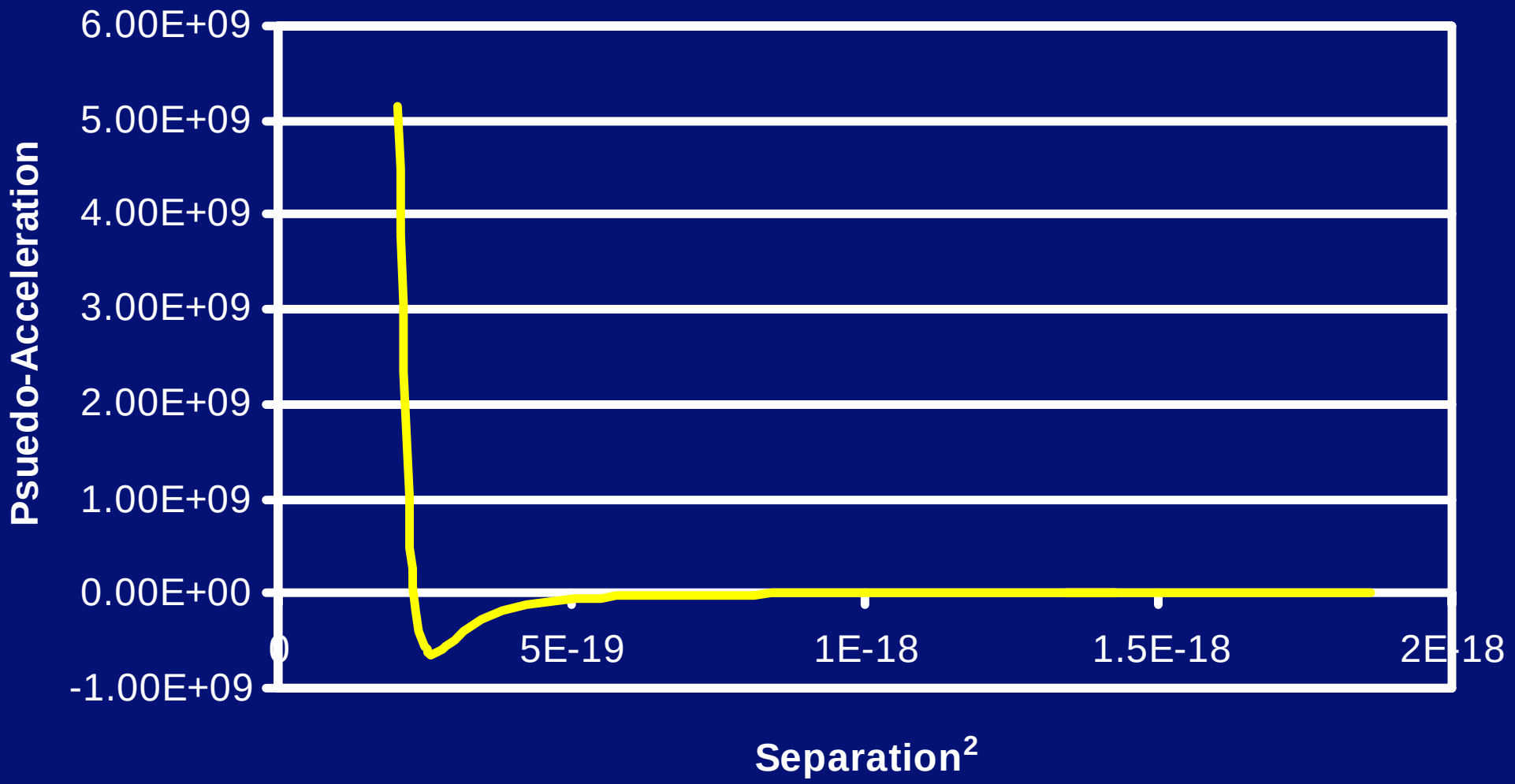
Architectural Design – Force Computer

- r^2 from PG used for function lookup
- Interpolate to obtain a more accurate force magnitude

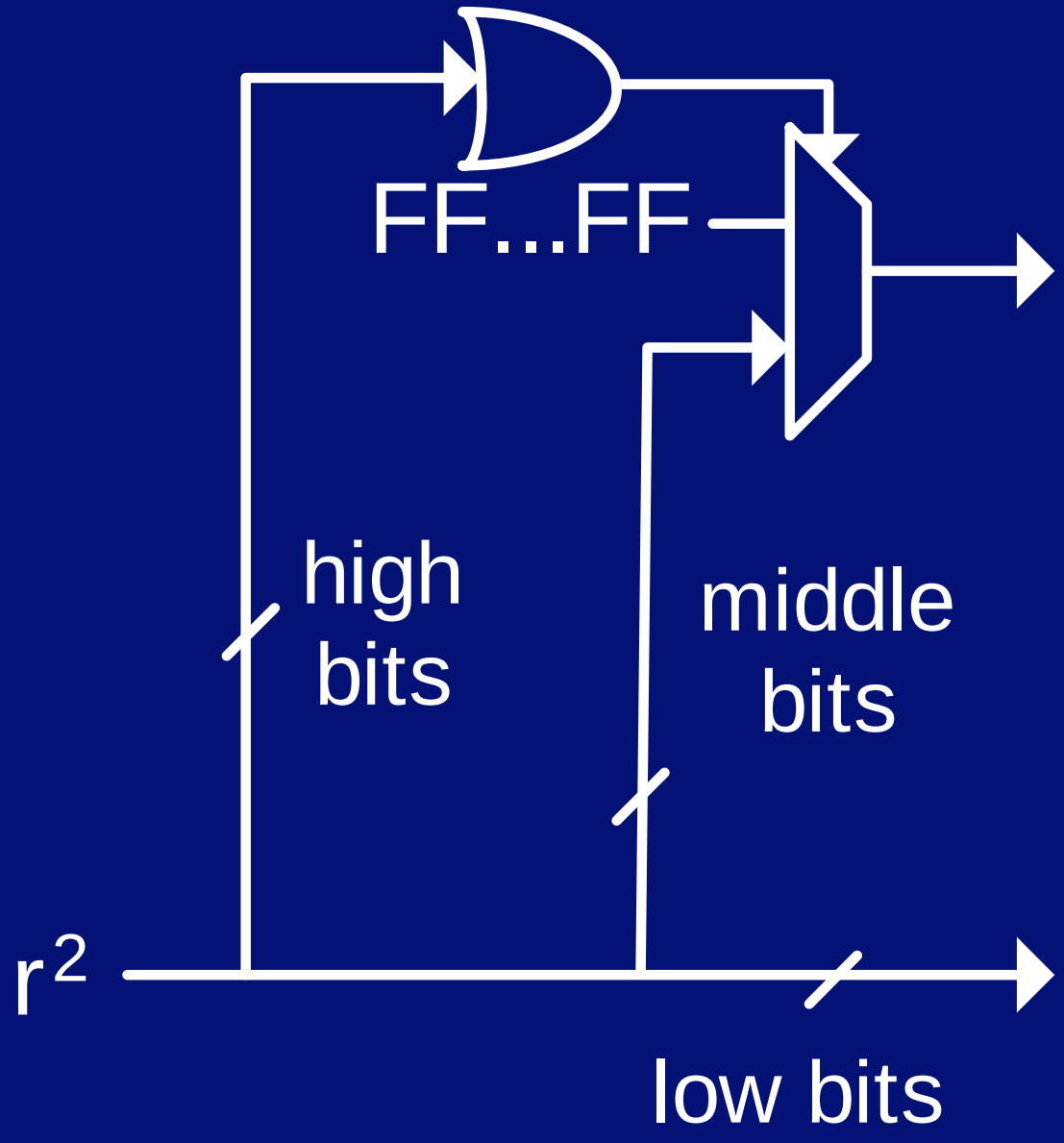


Architectural Design – Force Computer

- r^2 is larger than 18-bits
  - Look up table has a 18-bit address



Architectural Design – Force Computer



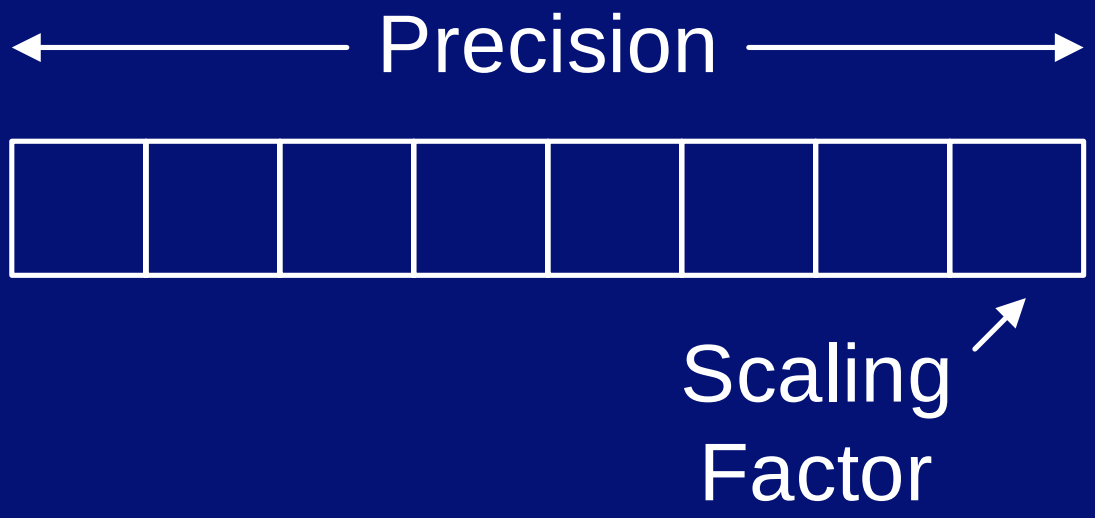
Address to lookup tables

Residual for interpolation

Precision and Scaling Factors

- Architecture uses integer operations to reduce complexity

- **Precision**: number of bits used to represent a value
- **Scaling Factor**: the weight of the least significant bit of the value



Calculating the Precision and Scaling Factors

- Calculations made with atoms at varying distances

- Scaling Factor = the minimum value
- Precision = $\log_2$ of the difference between minimum and maximum

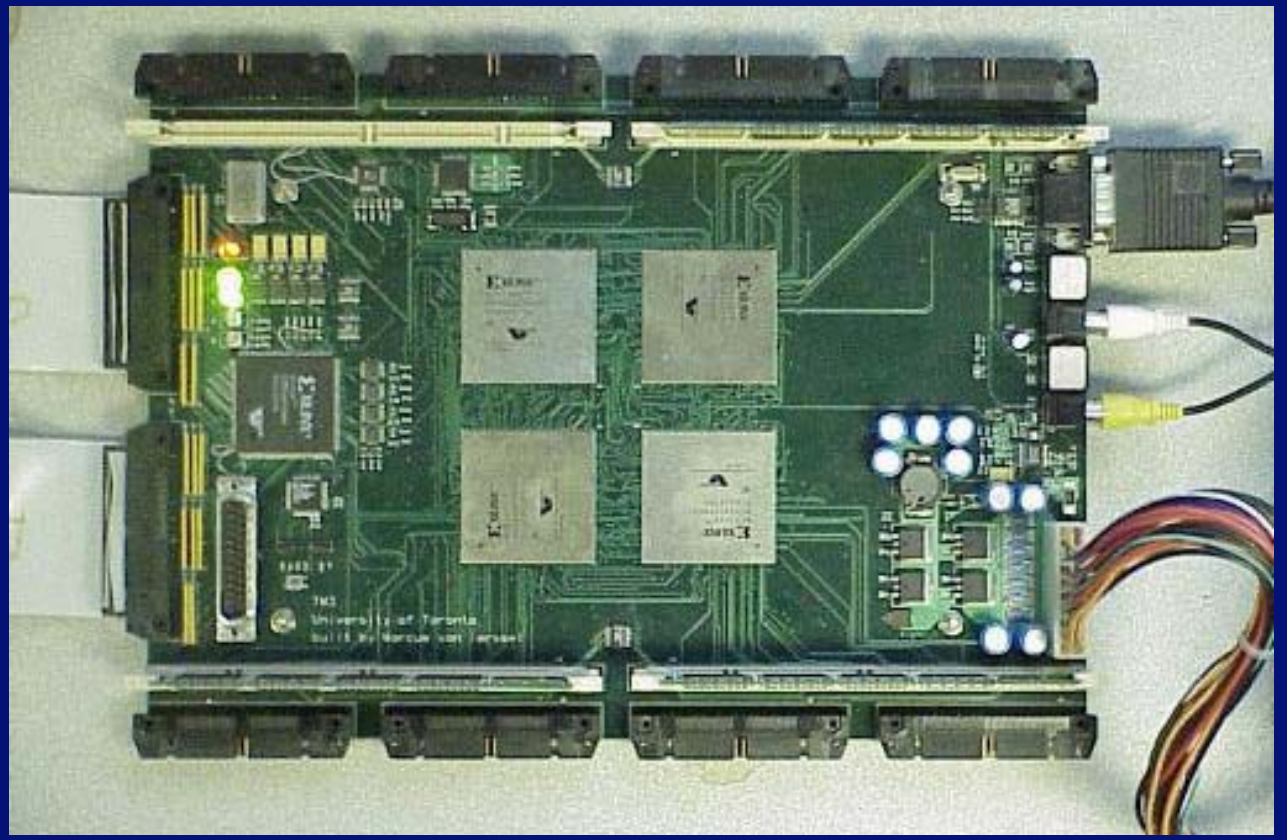
Quantity	Scaling Factor	Precision
Position	2^{-64}	38
Velocity	2^{-15}	51
Acceleration	2^{-64}	37

Simulation Environment is Configurable

- Simulation reconfigurability
  - Change precision, scaling factors, number of atoms. forces
  - No wasted hardware
  - No time overhead when precision is reduced
- Entire process is automated
  - One input file controls entire process
    - Hardware
      - C program creates appropriate VHDL
    - Software interface, Software initialization
      - Always match the hardware

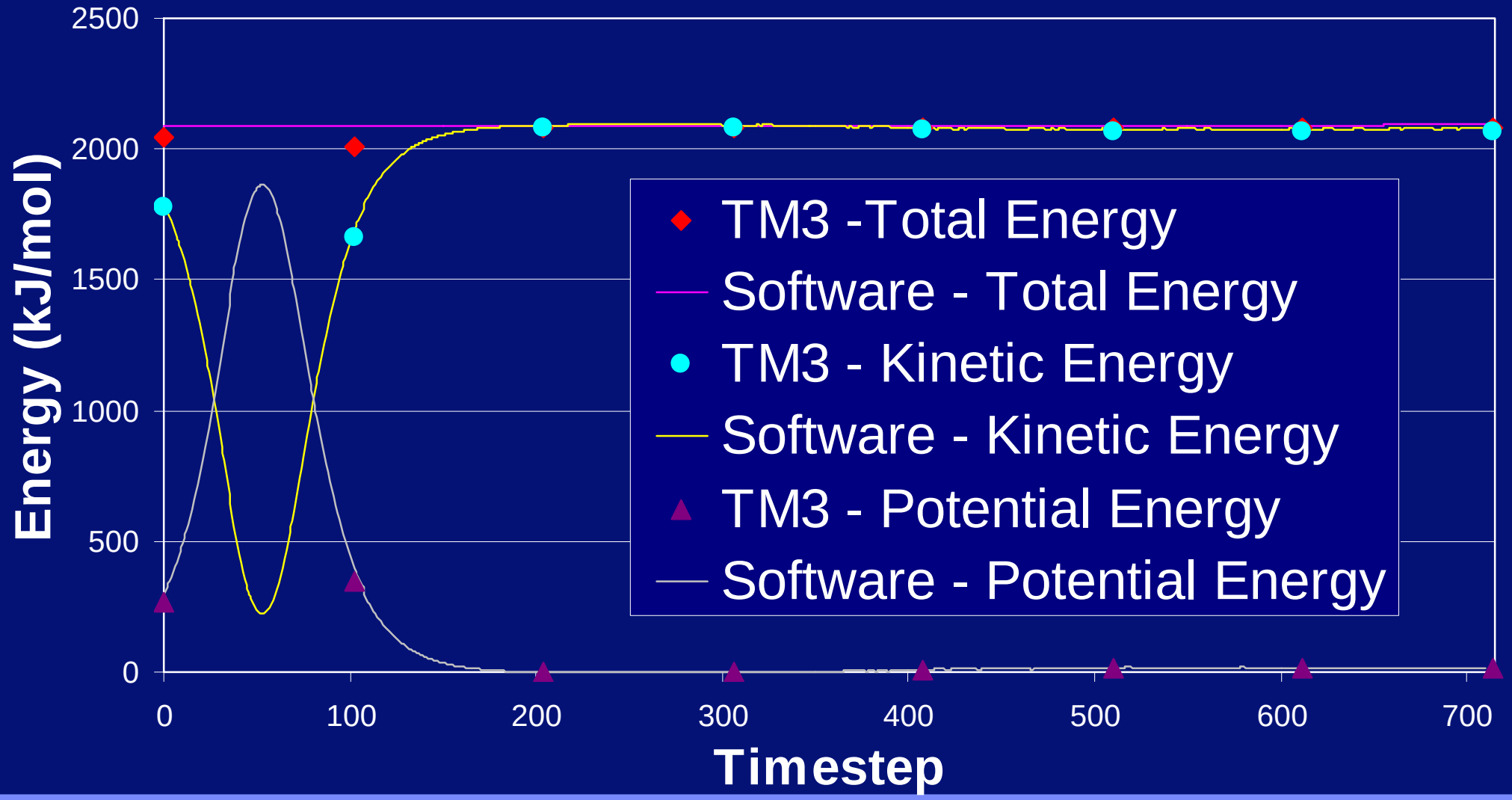
Implementation

- Used the Transmogrifier 3
  - –4 interconnected Virtex-E 2000's
  - –2MB memories connected to each Virtex-E
  - –Slow by today's standards



Verification

- Tested accuracy of implementation
  - Compared TM3 results with software



System Performance

- For a 8192 atom MD system running on the TM3
  - Frequency: 26 MHz
  - Timestep Duration: 37 sec
- For a 8192 atom software system running on a 2.4GHz Pentium 4
  - Timestep Duration: 10.8 sec
- MD system is 3.4X slower than software

How to improve this?

- Memory
- New FPGA
- Parallelism

Memory Requirements of MD System

- Acceleration Array (8192 atom system uses 0.17 MB)
- Velocity Array (8192 atom system uses 0.17 MB)
- Position Array (8192 atom system uses 0.34 MB)
- Lookup Tables: 2 MB

Improving Performance – Memory Organization

- On TM3 there is only one external SRAM per FPGA
- Single SRAM for all atom information causes large slowdowns
  - Handshaking
  - Serial reads for x, y and z
  - Hardware issues

Better memory system

2.1 seconds/timestep (5X faster than software)

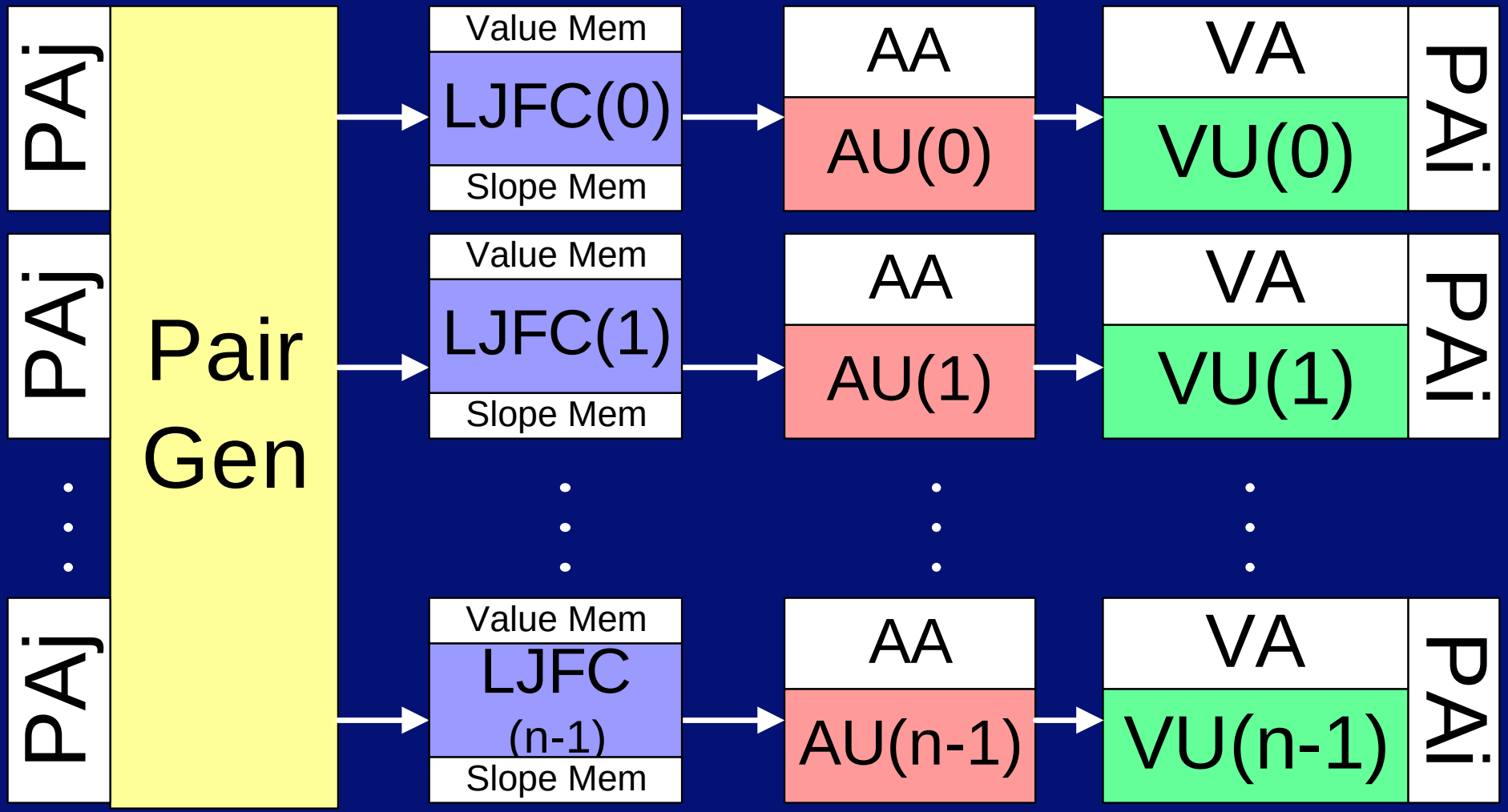
Improving Performance – Clock Speed

- Run on modern FPGA
- All possible improvements for clock speed not explored
- Expect a factor of 4 increase to a 100MHz

Better memory system + Faster Clock Speed

0.51 seconds/timestep (21X faster than software)

Improving Performance – Parallel Architecture



Better memory system + Faster Clock Speed + Parallelize

0.51/n seconds/timestep (21n X faster than software)

Cost, Power Benefits

- Performance
  - MD system can deliver a 21X performance benefit over software
  - Assume a conservative 10X performance advantage
- Cost
  - Microprocessor motherboard-sized board can fit 4 FPGAs
  - 4 FPGAs (each $200) + board + SRAM + misc. ~ $1500
  - Microprocessor Motherboard + CPU + DRAM ~ $1500

Comparison of MD Simulator and Supercomputers

Per Board	1 Pentium + 1 GB DRAM	4 FPGAs + 24 MB SRAM
Performance	1X	40X
Cost	~$1500	~$1500
Power	106W	40W

Metric	Improvement of MD System
Performance/Power	100X Improvement
Performance/Cost	40X Improvement
Performance/Space	40X Improvement

Conclusions

- Easily reconfigurable MD System designed
- Molecular dynamics simulation can be done on FPGAs
- Simple enhancements will improve speed
  - Power, Cost and Space savings over software

Future Work

- Improve accuracy
- Target newer FPGA platform
- Support new forces

Acknowledgements

- Funding for the TM3 Project was provided by Micronet and Xilinx