**Motivation**

• Computer simulations of biomolecules is increasingly playing an important role in medical research.
• Understanding the balance of physical forces governing atomic-level interactions is a central challenge in modern biochemistry.
• Computer simulations have been successfully applied to study physiological phenomena including:
  - Cell membrane transport.
  - Molecular conformational equilibrium.
  - Protein-Ligand docking.
  - Time-dependent molecular motion.
• Current technological limitations restrict the size and length of simulations.
• The primary objective of this study is to engineer a scalable Molecular Dynamics simulator which is capable of outperforming supercomputers and computing clusters.
• This project is a collaboration between the Department of Electrical and Computer Engineering, University of Toronto and the Department of Structural Biology and Biochemistry, The Hospital for Sick Children.

**Force Calculations ($F = - \nabla U$)**

\[
E_{\text{bond}} = -k_\text{bond} (r - r_0)^2
\]

\[
E_{\text{angle}} = -k_\text{angle} (\theta - \theta_0)^2
\]

\[
E_{\text{hinge}} = -k_\text{hinge} \left( \mathbf{r} \cdot \mathbf{r} - r_0^2 \right)
\]

\[
E_{\text{vanderWaals}} = 4 \varepsilon \left( \frac{\sigma}{r} \right)^{12} \left( \frac{1}{r} \right)^6
\]

**Molecular Dynamics Architecture**

- **Coordinate Repository**: Stores the coordinates of all atoms.
- **Compute Force**: Calculates the forces on each atom.
- **Integrate Forces**: Integrates the forces to update the velocities and positions.
- **Reduce Forces**: Reduces the forces and sends them to the output.

**Conventional vs. Proposed Implementations**

- **NAMD**: A state-of-the-art MD program, employs many techniques to improve simulation performance including:
  - Serial MD algorithms.
  - Parallel MD algorithms.
  - Ewald Electrostatic Force Engine.
  - Serial Protocol enables a fully-distributed implementation.

- **Our proposed implementation is not another attempt at building a supercomputer. This is an interdisciplinary effort to design a machine that performs MD simulations many times faster than the current supercomputer-based approach.**

**Hardware Components**

- **First Generation Prototype**
  - Field Simplex Links abstract on-chip hardware communication
  - Standard interfaces enable modular integration of system modules
  - Heterogeneous mixture of processors and accelerators

- **Second Generation Prototype**
  - Multi-Gigabit Transceivers allow gigabit-rate communication
  - Serial Protocol enables modular integration of system modules
  - High integration density possible

**Hardware Prototypes**

- **First Generation Prototype**
  - An integrated circuit board of 2,3 computing cores
  - Slow Simplex Links abstract on-chip hardware communication
  - Standard interface enables rapid chip communication
  - Multi-Gigabit Transceivers allow gigabit-rate communication
  - FPGAs combine computation and communication hardware on-chip

- **Second Generation Prototype**
  - An integrated circuit board of 32,3 computing cores
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