Stochastic Computing on GPUs

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What does a Protein Look Like?

- Several possibilities – spheres-only, ball-and-stick, sheets and ribbon representations, …

- *What does it look like to the solvent?*

![Crambin Smooth Molecular Surface [Richards 77]]
Ion Channels

- Proteins that regulate the flow of ions into and out of the cell membranes.

- Ion channels are highly specific cell filters.

- Ion channel transitions are very fast.

- Ion-channel-driven processes believed responsible for Alzheimer's disease, Parkinson's disease, epilepsy, schizophrenia, stroke, and cystic fibrosis.

- Understanding of ion-channels is vital for rational drug design — nearly a third of the top 100 pharmaceutical drugs target the ion-channels.

(from Alberts et al. 2003)
E. Coli Mechanosensitive Channel

EColi MsCL data from Sergei Sukharev (UMD) and Bob Guy (NIH)

Molecular surface  Surface Electrostatics
Ongoing Research: Salient Frames

Manifold Learning ideas using eigenanalysis to detect anomalous and representative frames in large molecular dynamics trajectories

Joint work with Patro, Kim, Ip, O’Leary, Anishkin, Sukharev, Hyeon, Thirumalai
How is a molecular surface useful?

- Visualization — examining fit and complementarity.
- Useful in simulating the effect of the water molecule on a protein (use surface area and its derivatives)
  - studying the structure and interactions of proteins
  - prediction of 3D structures of biological macromolecules and assemblies
- Existing approaches compute triangulated molecular surface and then sum the areas of the triangles
- But what if you just want the surface area?
- And what if you have lots of processors to help?
Cauchy-Crofton Approach

• Stab a molecule and a known object (say a sphere) with lots of random lines

• Count the number of intersections for each

• Surface areas are proportional to intersections

Nice properties:

• Parallel, progressive, scalable, efficient

• Maps well to GPUs

Some care is needed in:

• Random sampling in the space of lines
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Choosing Random Sequences

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**Some care is needed in:**

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• Quasi-random Sequences for Efficiency
Stochastic sampling of PDB 1HTO: 10K (left), 100K (middle), 1000K (right)

- Gives a 40x to 80x improvement for comparable accuracy
- Rough estimate almost immediate with improvement over time

*Think of each thread processor as a stochastic process!*
Stochastic Processors for NanoAssembly

- Recently-funded NSF project with Satyandra Gupta (Mechanical Engg)
- Nanocomponent devices are expected to revolutionize health care, energy, communication, and computing.
- Prototyping at the nanoscale requires manipulation of nanocomponents using optical, electrostatic, or magnetic trapping fields.
Final Remarks

- Stochastic stream processing serves as a useful way to map several problems to modern many-core GPUs
  - Each processor by itself or a group of processors collaborate to synthesize a stochastic process
  - Ensembles of such stochastic processes yield useful time vs accuracy trade-offs
  - Potentially useful for perturbation analysis and Markov Chains
- Will be useful to further study how to fully realize the power of stochastic processing on GPUs