

Identifying DNA Nucleotides based upon Flight Times

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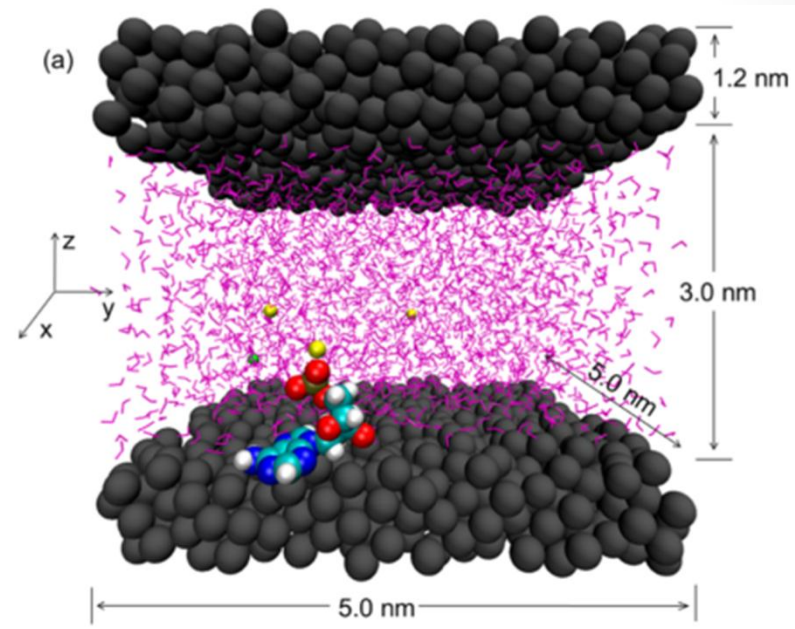
Goals of Research

Several Goals:

1. Develop a better understanding of Continuum Hydrodynamics and Molecular Dynamic Simulations
2. Work with MD simulations to determine the feasibility of identifying mononucleotides based on flight time through a nanoslit
3. Understand/investigate mechanisms and energetics of mononucleotides
 - Wall development

Project

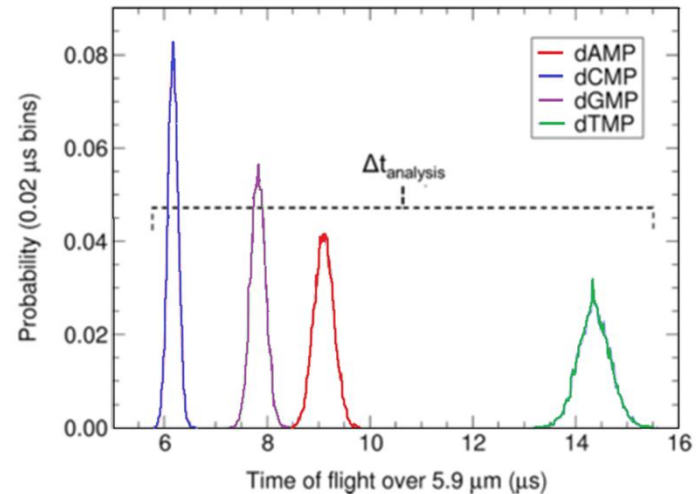
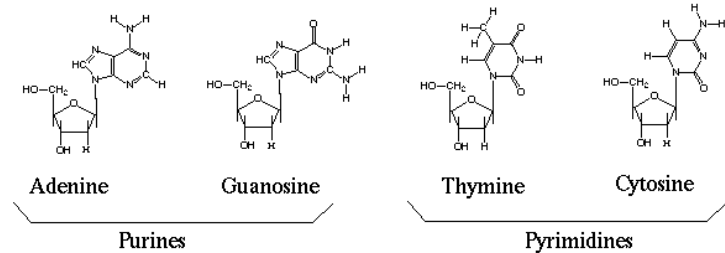
- Identify DNA nucleotides based on transit times over specified distance
- Need for new methods of genome identification
- Simulation Specifications:
 - Simulated DNA strand cut using λ -exonuclease
 - dNMPs with phosphate on 5' end
 - Length \approx 5.9 micrometers
 - Walls: Lennard Jones 12-6 parameters for carbon atoms
 - CHARMM Forces



Results/ Things Learned

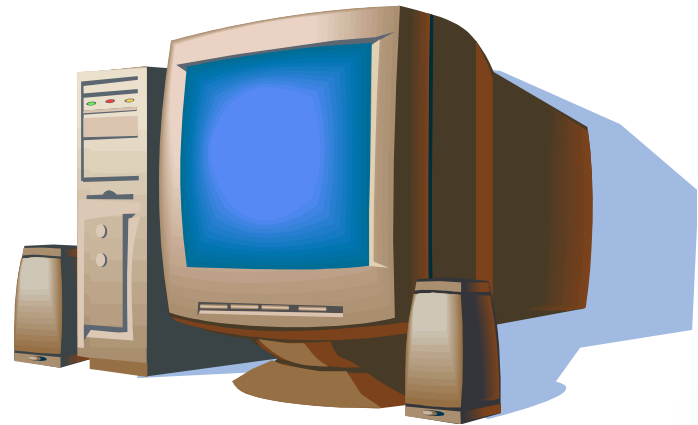
- Feasible to identify nucleotides via time of flight in nanochannel
 - Related to hydrophobic properties of nucleotide bases
 - Order of flight times (ns): C < G < A < T
- Walls need further manipulation
 - not replicable in lab setting
- Knowledge of interactions between fluid immersed particles and walls at molecular level

The Nucleotides of DNA

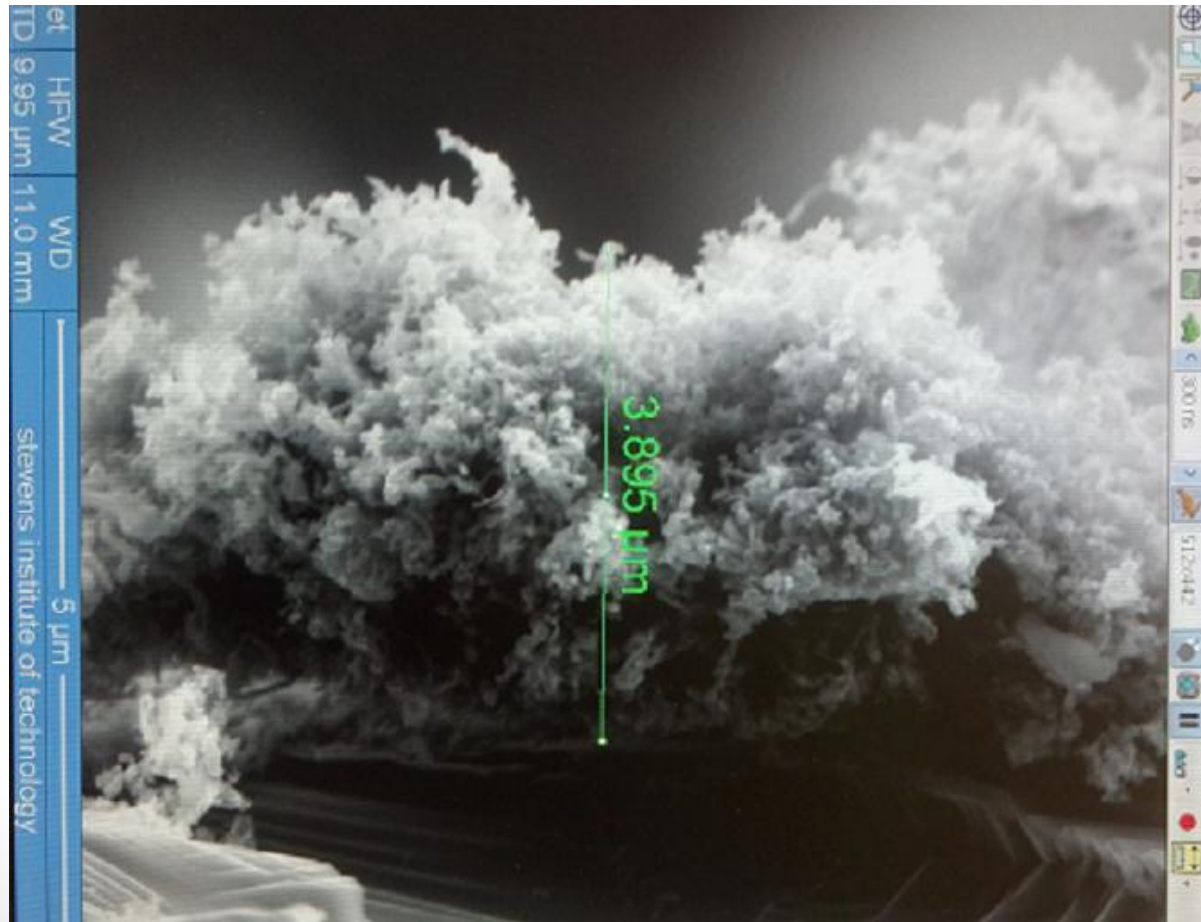


Challenges

- Understanding/working with new materials including:
 - Continuum Hydrodynamics
 - Linux/GROMACS MD/ VMD



Future Plans



Acknowledgments

- LA-SiGMA program
- Louisiana Board of Regents
- National Science Foundation

