

Big Data in the Big City

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- City University of New York
- Research examples
- Challenges
- Future plans



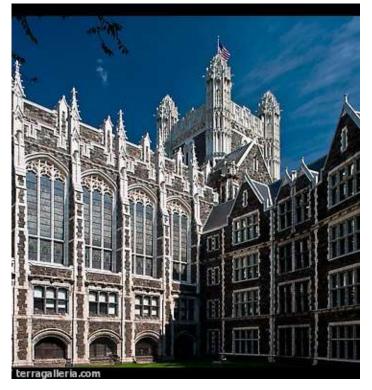
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- NYC Council through the efforts of Councilman James Oddo
- Borough President of Staten Island James P. Molinaro
- New York State Regional Economic Development Grant

HPCC MISSION STATEMENT

- Support CUNY's "Decade of Science" Initiative and the Integrated University Concept of Operation.
- Support the University's research and educational activities by making state-of-the-art HPC resources and expert technical assistance available to faculty and students.
- With CUNY faculty and researchers, develop proposals for external funding.
- Support National, New York State, and New York City initiatives in economic development.
- Support National and New York State initiatives to promote the sharing of HPC resources and technical knowledge.
- Support educational outreach programs designed to encourage intermediary and high school students to pursue higher education and careers in science and technology.

CUNY - Background



Senior Colleges

- City College
- Hunter College
- Baruch College
- Brooklyn College –
- Queens College
 Lehm

- New York City College of Technology
- College of Staten Island
- John Jay College of Criminal Justice
- e York College
- e Lehman College
 - Medgar Evers College

- Community Colleges
 - Bronx Community College
 - Queensborough Community College
 - Borough of Manhattan Community College
 - Kingsborough Community College
 - LaGuardia Community College
 - Hostos Community College
 - New Community College
- Graduate and Professional Schools
 - CUNY Graduate Center
 - Sophie Davis School of Biomedical Education
 - School of Law
 - William E. Macaulay Honors College
 - Graduate School of Journalism
 - School of Professional Studies
 - School of Public Health



- Largest urban university in the United States
 - 271,000 degree program students.
 - 270,000 adult, continuing, and professional education students.
- Gender
 - 61% female
 - 39% male
- Ethnicity
 - 0.2% American Indian/Native Alaskan
 - 15.8% Asian/Pacific Islander
 - 27.1% Afro-American
 - 25.7% Hispanic
 - 31.2% White
- 72% attended New York City public high schools
- 42% first time freshman
- 32% work for pay more than 20 hours per week
- 189 different languages spoken as first language

CUNY - Alumni

Nobel prize winners

- Julius Axelrod
- Kenneth Arrow
- Robert Aumman
- Stanley Cohen
- Gertrude Elion
- Herbert Hauptman
- Robert Hofstader
- Jerome Karle
- Henry Kissinger
- Arthur Kornberg
- Leon Lederman
- Arno Penzias
- Julian Schwinger
- Rosalyn Sussman Yalow

- Fields Medal winners
 - Jesse Douglas
 - Paul Cohen
- Felix Frankfurter, Supreme Court Justice
- Celina Sotomayer, mother of Supreme Court Justice Sonia Sotomayer
- The parents of Michael Dell
- The parents of David Bader
- Dr. Jonas Salk, Polio Vaccine
- Robert Kahn, Co-developer of TCP/IP
- Andy Grove, co-founder and former CEO, Intel Corp.



Located at the College of Staten Island

Welcome to the College of Staten Island, City University of New York.



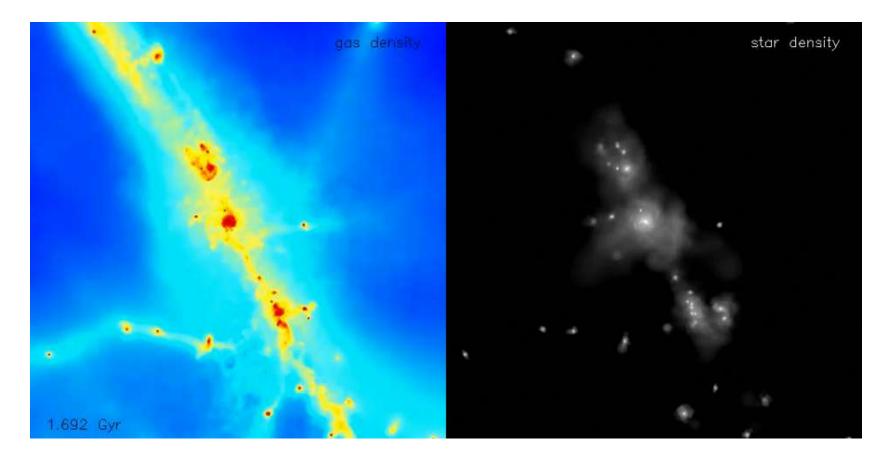




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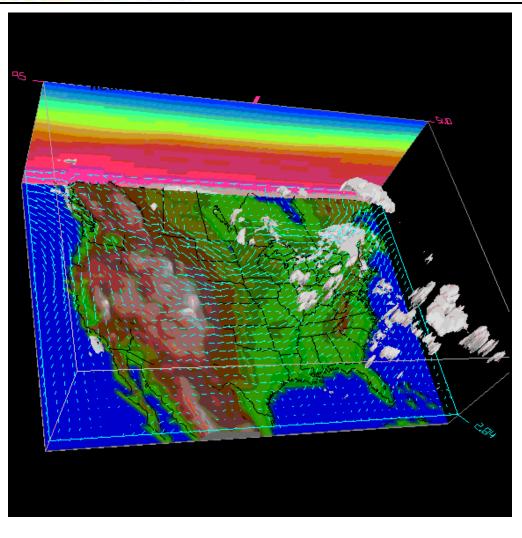


Simulation of a Single Galaxy *



* Computational cosmology: The evolution of the galaxy Courtesy: Dr. Ari Maller, New York College of Technology/CUNY

Environmental Science



- Numerical Weather Prediction/Climate Modeling
 - Ocean models
 - Terrain
 - Vegetation
 - Chemicals
 - Particulates
 - Hydrology
 - Human impact

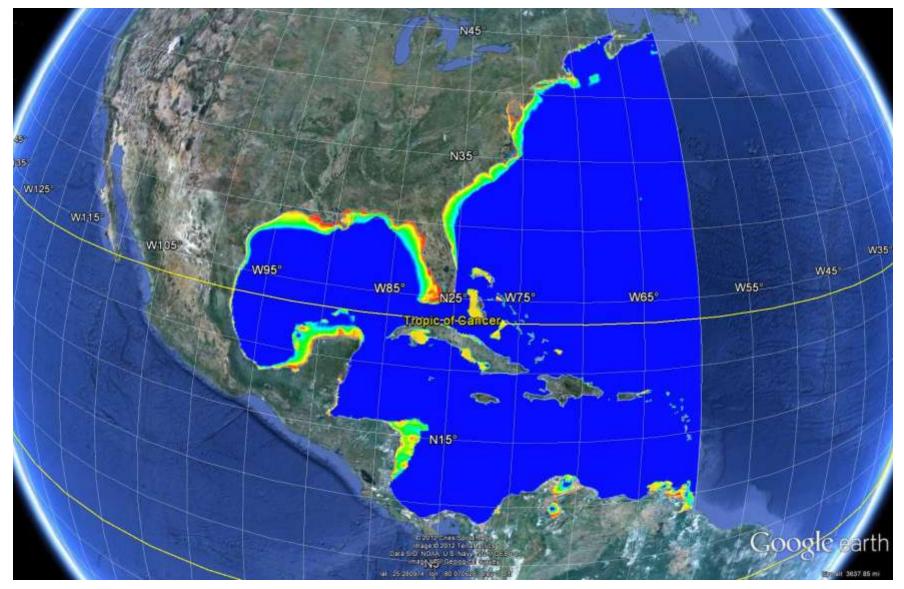
CUNY Collaborative Remote Sensing Systems Technology Institute & the CUNY Environmental CrossRoads Initiative

July 10, 2012

11

11

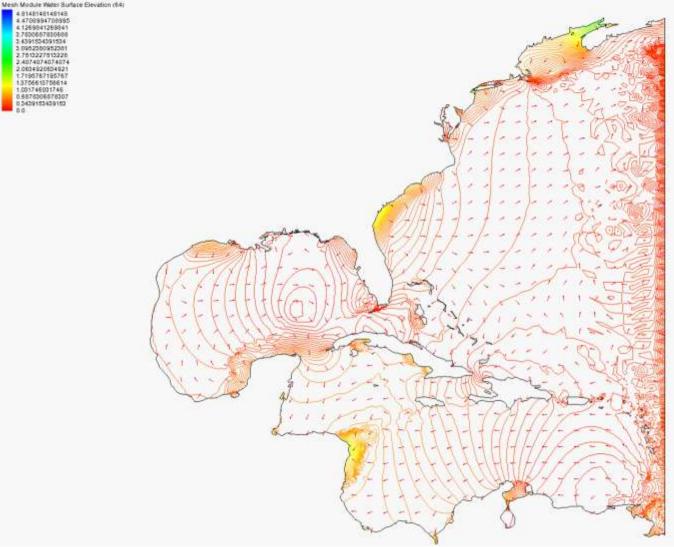
Coastal and Estuary Modeling





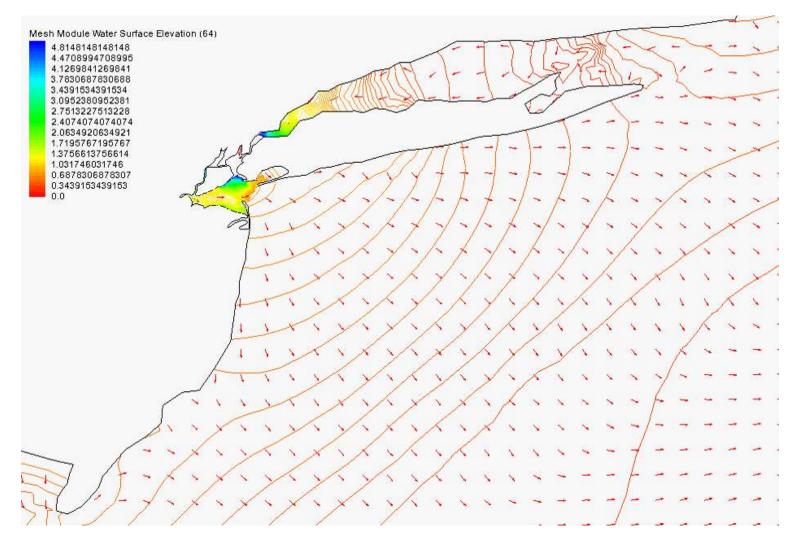
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Coastal and Estuary Modeling*



* Courtesy: Dr. M. Kress, et al, College of Staten Island





Coastal and Estuary Modeling



Deep Water Horizon *

31°N

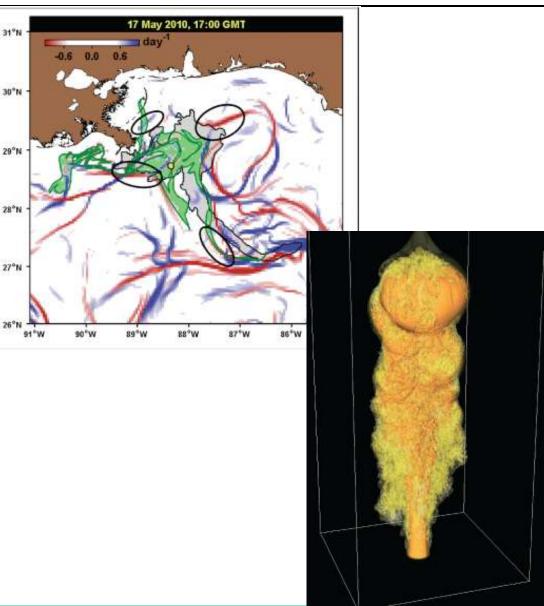
30°N

28°N

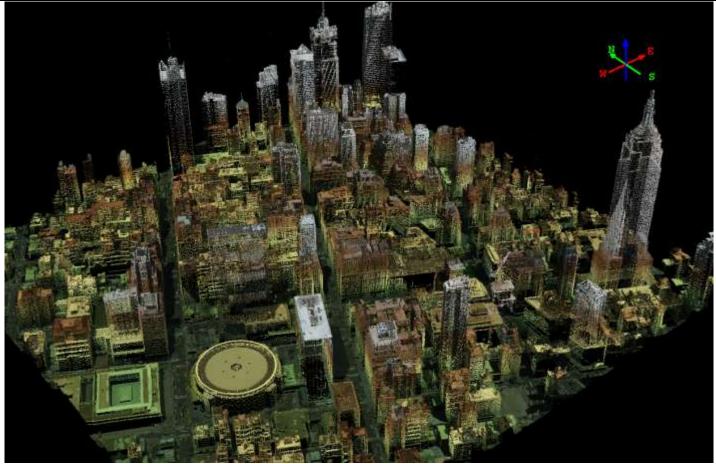
27°N

Hydrocarbon Transport

- Huge range of scales
 - 1 U surface layer
 - O(10 m) plume
 - O(100 km) eddies
 - Tidal & Surf zones
 - Multi-scale turbulence •
- **Evovling Physio-Chemistry** •
 - Complex chemistry
 - Biology ٠
 - Photo-chemistry ٠
 - Air-sea interactions •
- **Deep Ocean Processes** ٠
- * Courtesy: D. Poje, CSI/CUNY



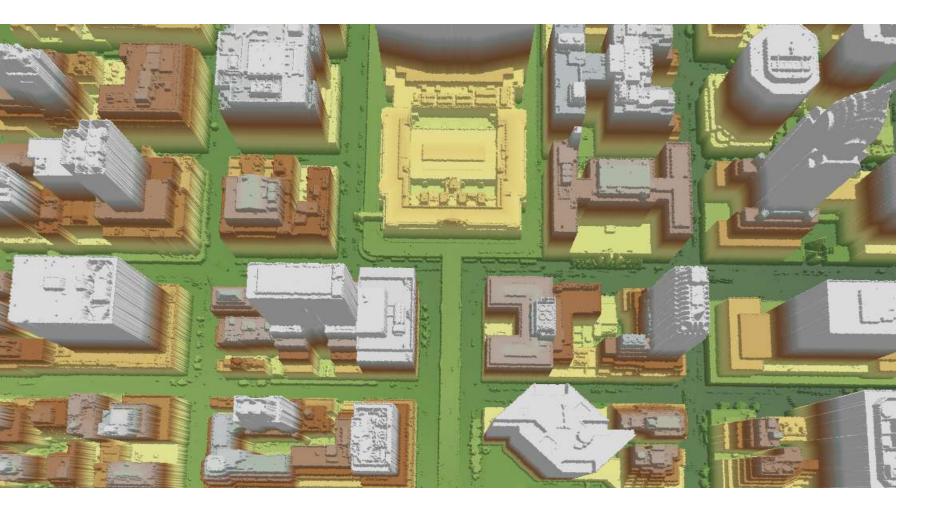
NYC SOLAR MAP *





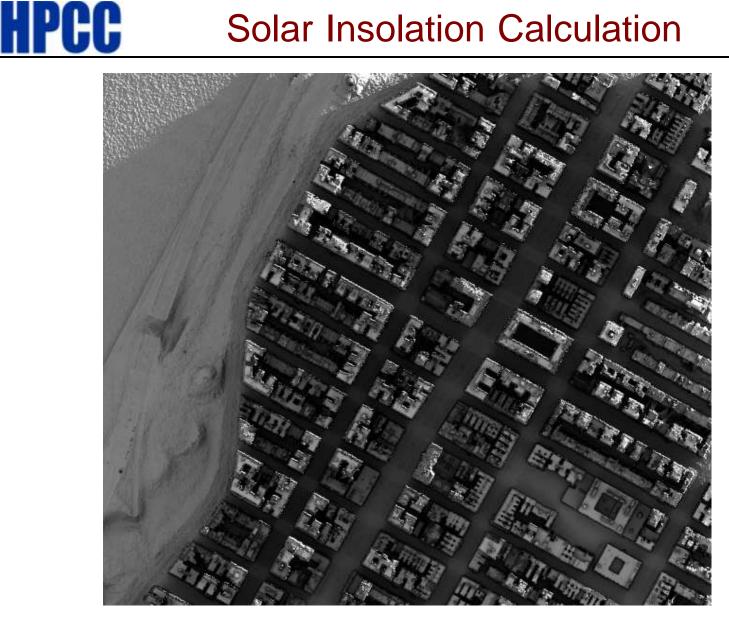
* Courtesy: Center for Advanced Research in Spatial Information, Sean Ahearn, et al, Hunter/CUNY

Points to Digital Surface Model (DSM)

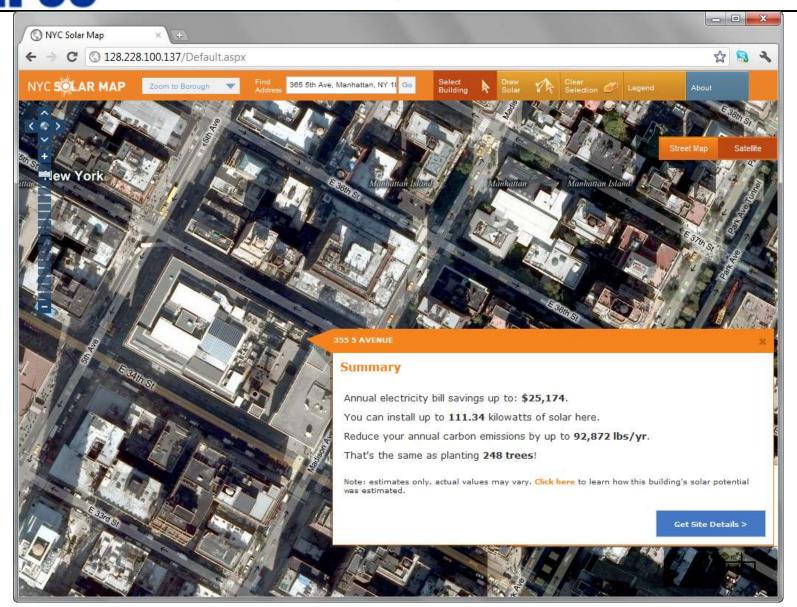


Technique 2: Adaptive triangulation with smoothing filter by 1 bin size radius and maximum g tolerance 3 meter, spike and well removal

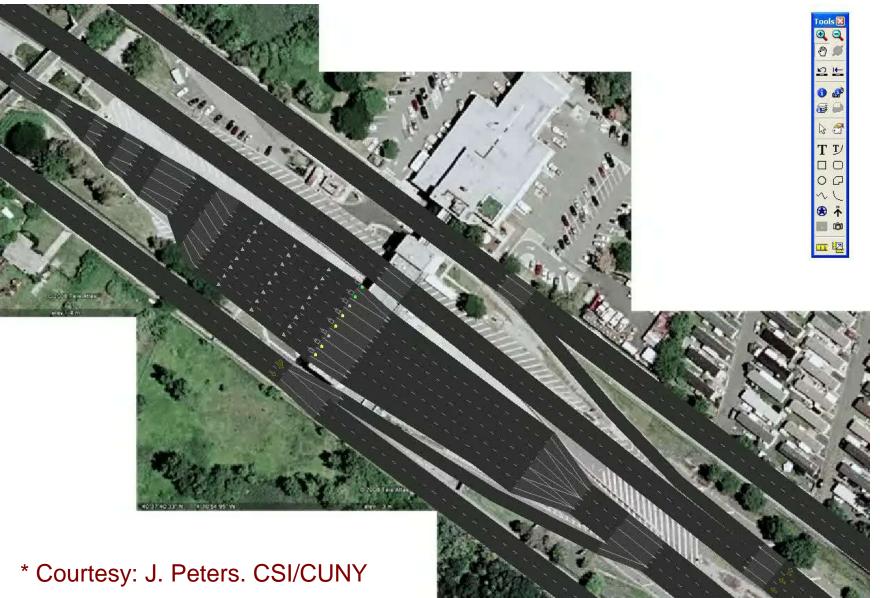
Solar Insolation Calculation



www.http://nycsolarmap.com



Traffic Studies *



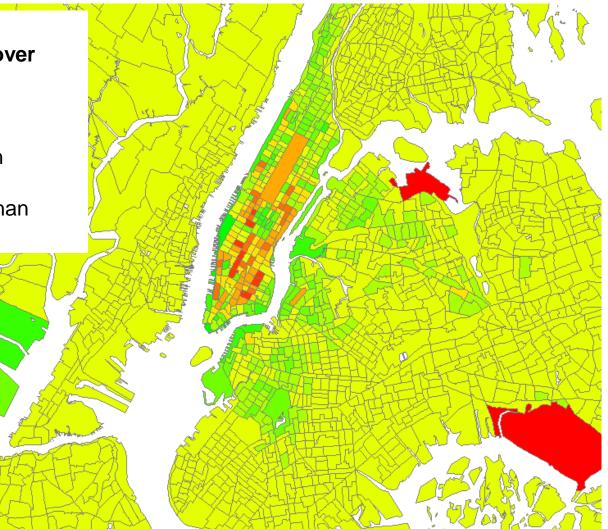


GPS tracking of taxi trips 378,532,118 observations over 18 month period

Red = More originations than destinations Green = More destinations than originations

* Courtesy:

D. King, Columbia UJ. Peters, CSI/CUNYC. Gordon, U of Canberra





Transportation Policy *

NEW YORK CITY TAXI ACTIVITY ORIGIN AND DESTINATION DENSITIES

Red = More originations than destinations Green = More destinations than originations * Courtesy
D. King, Columbia U
J. Peters, CSI/CUNY
C. Gordon, U of Canberra

Transportation Policy

Easypay usage

3 billion rides per year

Potential tracking of individual; user travel patterns

Linked to credit card

Posted Date	Transaction Date & Time	MetroCard Number	Ride Location	Transaction	Amount	Balance	Description
06/26/12	06/25/12 21:06:00	2228065429	R126 CHRISTOPHER ST SUBWAY	Ride: Subway	\$1.10	\$40.10	EasyPay Reduced Fare Plan
06/26/12	06/25/12 18:30:00	2228065429	R232 33 ST SUBWAY	Ride: Subway	\$1.10	\$41.20	EasyPay Reduced Fare Plan
06/26/12	06/25/12 12:06:00	2228065429	A069 CHAMBERS ST SUBWAY	Ride: Subway	\$1.10	\$42.30	EasyPay Reduced Fare Plan
06/22/12	06/22/12 20:52:42	64		Bonus	\$2.45	\$43.40	Reduced Fare
06/22/12	06/22/12 20:52:42	10		Payment Received	\$35.00	\$40.95	Reduced Fare
06/22/12	06/21/12 18:48:00	2228065429	R103 RECTOR ST SUBWAY	Ride: Subway	\$0.00	\$5.95	EasyPay Reduced Fare Plan
06/22/12	06/21/12 18:12:00	2228065429	X10 EXPRESS	Ride: Express Bus	\$5.50	\$5.95	EasyPay Reduced Fare Plan
06/18/1 <mark>2</mark>	06/17/12 21: <mark>36:0</mark> 0	2228065429	R138 34 ST-PENN STA SUBWAY	Ride: Subway	\$1.10	\$11.45	EasyPay Reduced Fare Plan
06/15/12	06/14/12 22:12:00	2228065429	Q30	Ride: Bus	\$1.10	\$12.55	EasyPay Reduced Fare Plan
06/12/12	06/11/12 18:42:00	2228065429	N083 W 4 ST-WASH SQ SUBWAY	Ride: Subway	\$1.10	\$13.65	EasyPay Reduced Fare Plan
06/12/12	06/11/12 17:54:00	2228065429	R103 RECTOR ST SUBWAY	Ride: Subway	\$0.00	\$14.75	EasyPay Reduced Fare Plan
06/12/12	06/11/12 17:12:00	2228065429	X10 EXPRESS	Ride: Express Bus	\$5.50	\$14.75	EasyPay Reduced Fare Plan
06/07/12	06/06/12 21:06:00	2228065429	A046 CANAL ST SUBWAY	Ride: Subway	\$1.10	\$20.25	EasyPay Reduced Fare Plan
06/07/12	06/06/12 18:30:00	2228065429	A060 WHITEHALL ST SUBWAY	Ride: Subway	\$1.10	\$21.35	EasyPay Reduced Fare Plan
06/05/12	06/04/12	2228065429	X10 EXPRESS	Ride: Express Bus	\$1.65	\$22.45	EasyPay Reduced Fare Plan

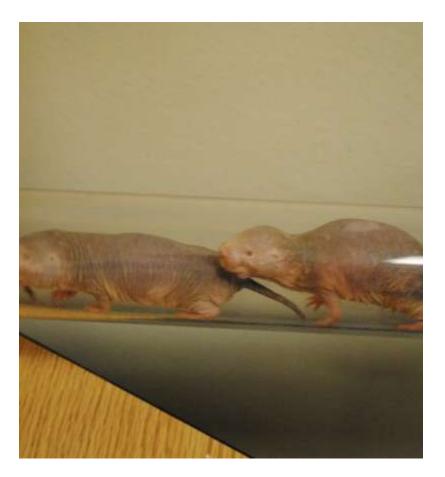








- Multi-level study of a "society" and its individual members
- Naked African mole rats
 - Not a mole
 - Not a rat
 - The only cold blood mammalian species (closest relative is the porcupine)
 - Offspring will likely never reproduce (less than 5% chance)
 - Genetically homogenous population
 - Life expectancy greater than 30 years
 - Skin is not sensitive to pain
 - Not known to ever develop cancer
 - Navigate using magnetic fields
 - Males and females are barely distinguishable
 - Communicate through chirps
 - Have individual recognition



* Courtesy; Dan McCloskey, College of Staten Island/CUNY

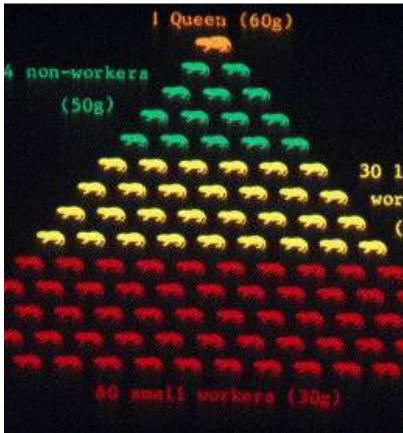


Structured society

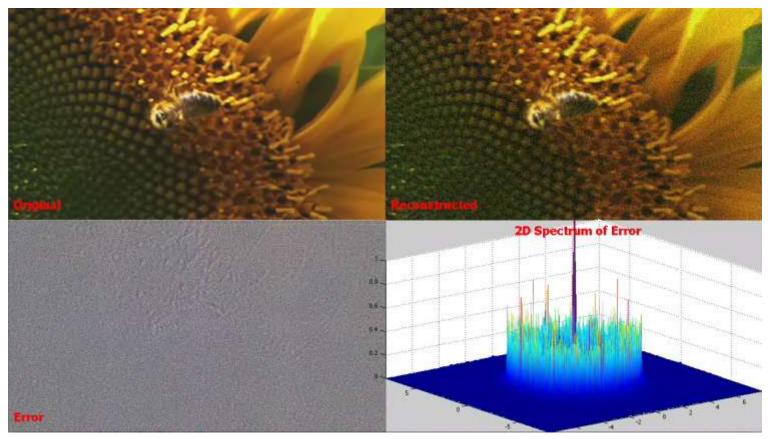
- Only the queen has off-spring
- Tunnel diggers
- House keepers
- Food gatherers
- Exclusive society
- Instrumented
 - RFIDs to capture movement and social interactions
 - Monitor communications
 - Monitor oxytocin levels/blood chemistry
 - Brain structure analysis (MRI and biopsies)

Longitudinal studies over time

- 100s of millions of data points
- Social graphs
- Correlate social interaction/social position with:
 - Structure of neuronal circuits
 - Oxytocin levels



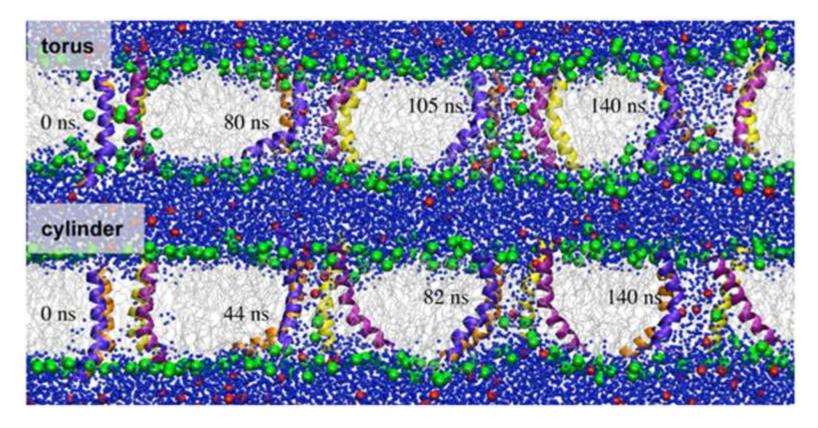
Courtesy; Dan McCloskey, College of Staten Island/CUNY



Emulating the neural encoding and decoding circuits of the early vision system

* Courtesy: Aurel Lazar, BioNET Group, Columbia University Computations using 55 GPGPU's on CUNY's Andy HPC system

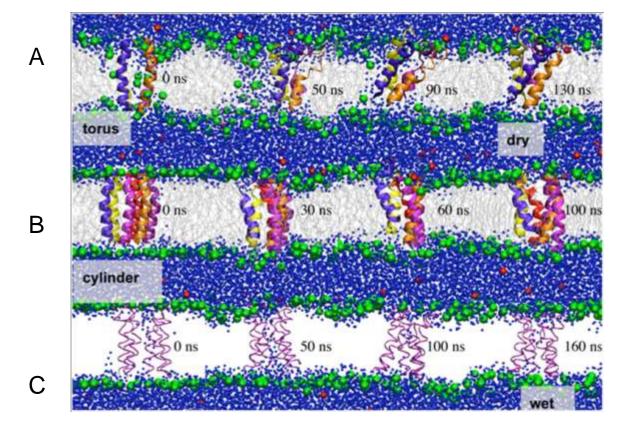
Using MD to Understand the Permeability of Cells *



Through this molecular dynamics calculation, we see that melittin preserved the toroidal pore shape or reshaped an initially barrel-stave pore into a semitoroidal pore. This indicates that the electrostatic interactions are stronger in toroidal shaped pores. In this figure, the green balls represent phosphocholines; the gray lines: lipid tails; red balls: Cl-ions; blue balls: water; cartoons: peptides.

* Courtesy Drs. M. Mihajlovic & T. Lazaridis, City College/CUNY

Using MD to Understand the Permeability of Cells



To have a pore, water has to stay inside the pore region ("wet" pore); otherwise the peptides form an aggregate and the pore dries up (or closes). In our simulations, the latter happened when Q7's were not located within the pore. Glutamine is a polar residue and thus important for providing the hydrophilic environment necessary to preserve the aqueous pore. These studies showed that alamethicin preserved the barrel-stave shaped pore. Here we see that Glutamine Q7 seems to be important for stabilizing a wet pore. The pore remained wet when the glutamine Q7's were initially located within the pore, but dried up in the simulation when the Q7's were not oriented towards the interior of the pore. In this figure, the green balls represent phosphocholines; gray lines: lipid tails; red balls: CI- ions; blue balls: water; cartoons (in (A) and (B)), ribbons (in (C)): peptides; in (C), the lipid tails are removed for clarity.



- Display excellent scalability
- GPU versions available
 - Amber
 - DESMOND
 - Gromacs
 - NAMD



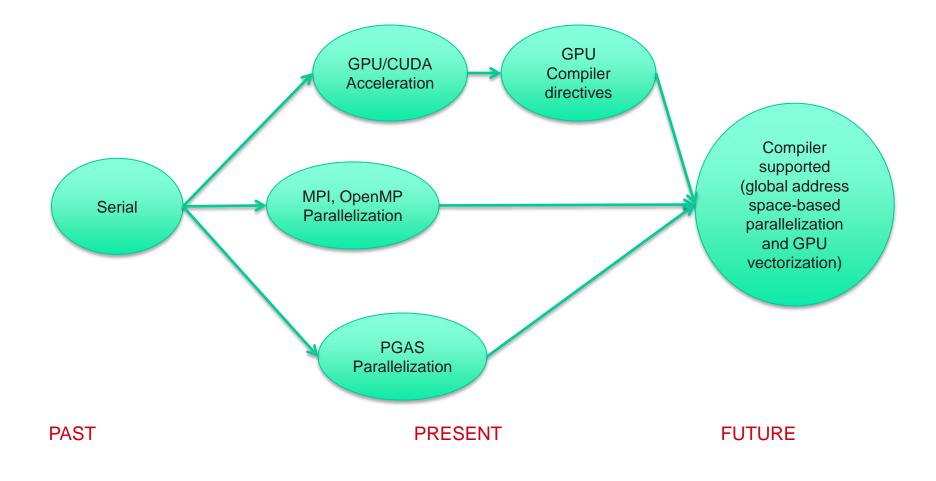
Sept 2012 Configuration

Syst em		Cores	Chip	Memory/core (GB)	Interconnect
Arno	Kepler ready	1,152	SandyBridge E5- 2660	2	QDR
Zeus	Gaussian	64	Harpertown	2	Ethernet
	Gaussian	16	Woodcrest	2	Ethernet
Bob	Gaussian	232	Barcelona	2	Infiniband
Andy	Serial & small parallel	744	Nehalem	3	DDR and QDR
	GPU	96 x 448	GPU - FERMI	3	PClex Gen2
SGI UV-2	Genomics Graphs	512	SandyBridge E5-4600	8 TB	SMP
Salk	Large scalable	2,816	Magny-Cours	2	Custom - Gemini
Karle		24	Westmere	96	SMP

Arno – Arno Penzias, physicist, Nobel Laureate Andy – Andy Grove, co-founder, Intel Karle – Jerome Karle, mathematician, Nobel Laureate Bob – Robert Kahn, co-developer TCP/IP

Salk – Jonas Salk, developer of the polio vaccine

HPC Philosophy/Vision



The HPCC has the state-of-the-art parallel HPC systems supporting the following programming models: OpenMP, MPI, GPU acceleration, and partitioned global address (Co-array Fortran and Unified Parallel C. This anticipates a future HPC trend leading to unified HPC programming models

- Application development is now more difficult, not less
- One computing architecture does not fit all
- Breakthrough research requires multi-disciplinary skills--universities are not meeting the challenge
 - Departments are stove-piped
 - Academic change is slow, change in technology is rapid
 - Pushing internal change is a key role of a university HPC Center
- New skills are required big data, semantic data, graph theoretic approaches
- Shortage of skilled people
- Universities lack computational resources
- Energy consumption per \$ spent on hardware has grown by an order of magnitude in 25 years



- Telescope
- Microscope
- Time machine

1025?



 Augmented with the help of HPC

New Facilities

- New 170,000 sq. ft. facility in planning stages
- 10,000 sq. ft. of raised floor
- Staff offices
- \$6.5 million committed for facility design
- Expected occupancy: 2017

