Accelerated Materials Discovery

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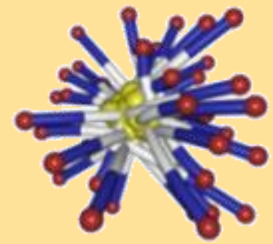
Accelerated Materials Discovery

New materials are essential for solving global challenges, and for the success of a wide variety of companies

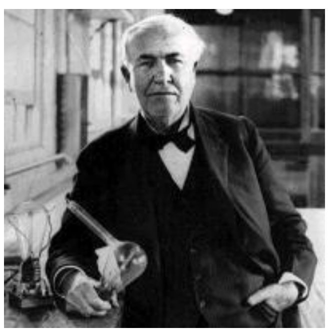
Smarter Planet: e.g. water filtration, recycling, low energy AC

Semiconductor: Nanotechnologies, chips



Life sciences: drug discovery, medical devices

Energy storage & generation: batteries, solar, CO_2



Expert-driven Trial and Error

Material Science

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Big Data

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Deep Analytics

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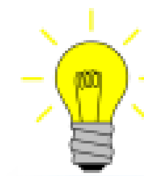
HPC

Combine domain knowledge, literature mining, experiments, simulations and analytics to increase the speed and decrease the cost of discovery.



Accelerated Discovery

Challenges include materials similarity, hypothesis generation, uncertainty, modeled vs. measured data, figure & table extraction, scalable infrastructure, domain customization

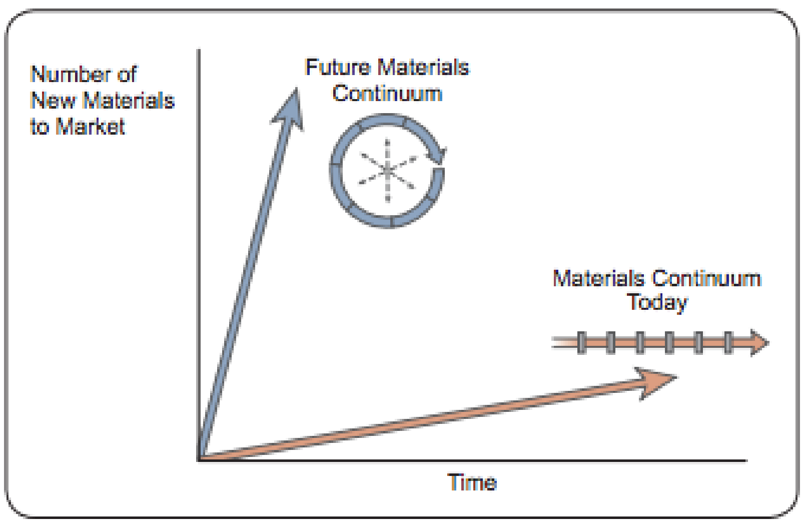
The Materials Innovation Life Cycle – White House Materials Genome Initiative
Investing $100M in 2012 alone across DOE, DOD, NIST, and NSF

From the White House Materials Genome Initiative for Global Competitiveness, June 2011

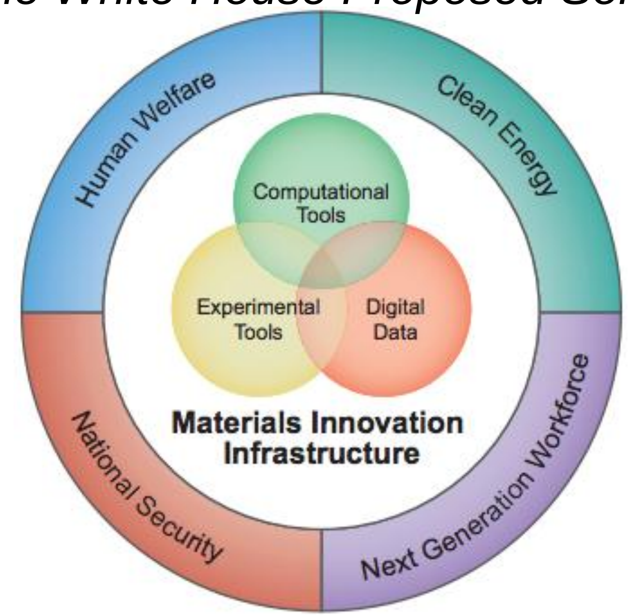
Discovery *Materials Development Continuum* *Deployment*

1 Research
2 Development
3 Property Optimization
4 System Design & Integration
5 Certification
6 Manufacturing
7 Launch

2x faster at a fraction of cost



The White House Proposed Solution



http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

Eras of Computing

Cognitive Systems Era

Programmable Systems Era

How do we get from here to there?

Tabulating Systems Era

Accelerated discovery is how we describe the next level of cognitive systems that are capable of addressing questions for which the answer is currently not known.

Computer Intelligence

Sorting and Counting | Processing and Coding | Learning and Reasoning

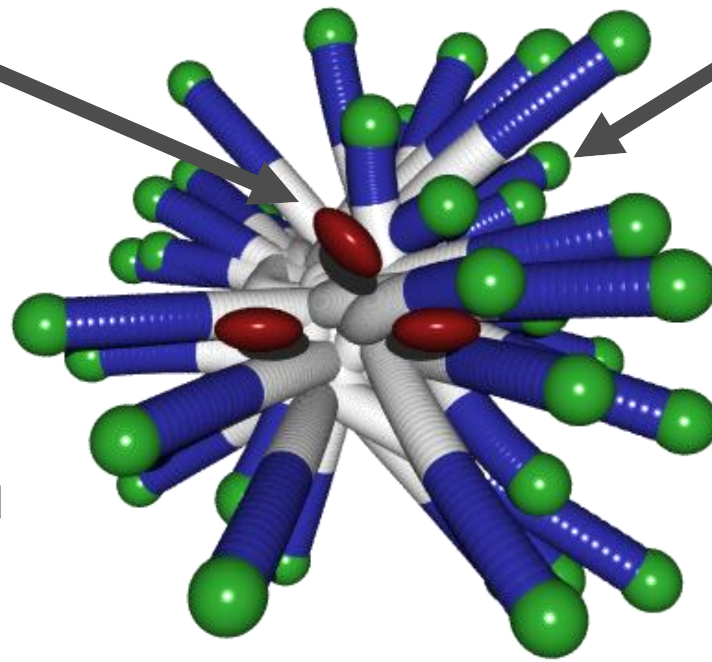
Time

Multifunctional Polymers for Therapeutic Delivery

Enhanced Micelles and NanogelCore-Shell Star-polymers

Core
(Cargo Encapsulation)

Shell
(Protection/Targetting)



- Biodegradable Core
- Enhance cargo loading
  - Hydrophobic drugs
- Release triggers
  - Disulfide
  - Schiff-base
- Directed self assembly and enhanced micelle stability

- Hydrophilic exterior
  - Poly(Ethylene glycol) PEG
  - PEG Alternatives
- Peripheral Functionality
  - Targeting peptides
- Responsive polymers
  - LCST polymers
  - pH responsive polymer

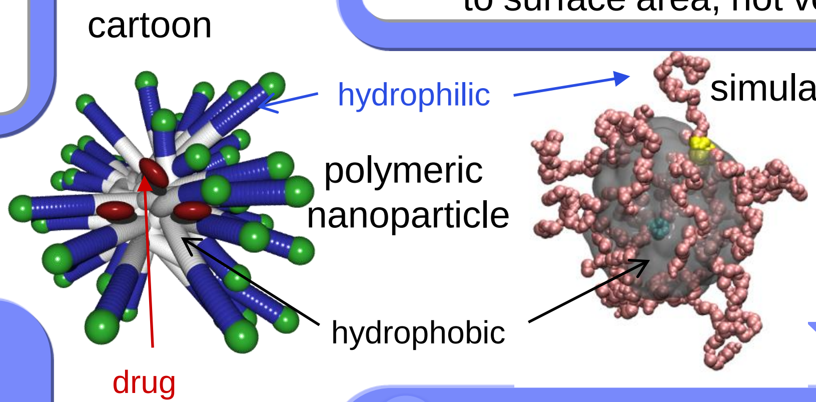
Scenario: Design a Superior Drug Delivery Vehicle

1 Chemists use Accelerated Materials Discovery (AMD) Platform to mine the literature

What drug delivery vehicles exist today?
What properties are important?
What are the problems?

2 Combination of literature knowledge with more information from simulations

Polymeric nanoparticle as potential vehicle
Simulations show drug uptake proportional to surface area, not volume -- why?



3 Polymer similarity search to suggest new "hydrophilic" & "hydrophobic" components; determine relevant properties "in silico"

Can these new polymeric nanoparticles be synthesized?

4 Ranked list of new polymers to make

Synthesize and test proposed polymeric nanoparticles in the lab

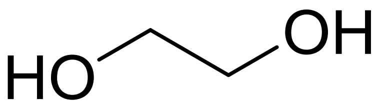
5 More information from experiment: polymeric nanoparticle aggregates; particles too large

Go back to literature or simulation
How is particle size controlled?
Alternative chemistries/architectures?

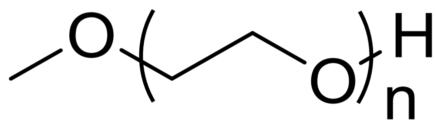
Specific Proposal

- To get started, we would like to process polymer data, in particular diagrams/figures of polymers. The OSRA open-source program http://sourceforge.net/apps/mediawiki/osra/ currently interprets diagrams of molecules (like ethylene glycol … but not polyethylene glycol)

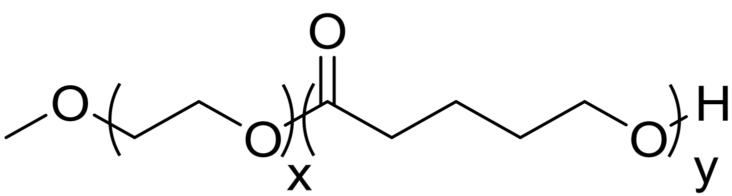
Ethylene glycol



Polyethylene glycol

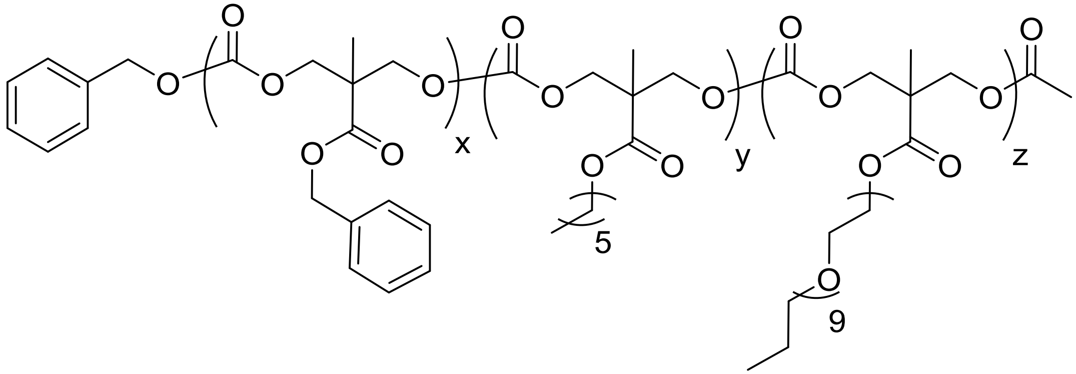


Polyethylene glycol-b-polyvalerolactone



- The program would need to be updated to
  - recognize ($)_n$ notation
  - form 3 chemical structure files (instead of one): one corresponding to the chemical structure within the square brackets; one corresponding to the CH_3O- end group, and one corresponding to the -H group

- As you can imagine, polymer structures can get progressively more complicated ….

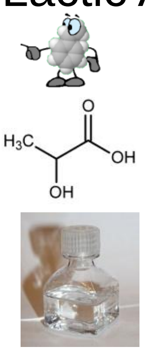


Project Requirements

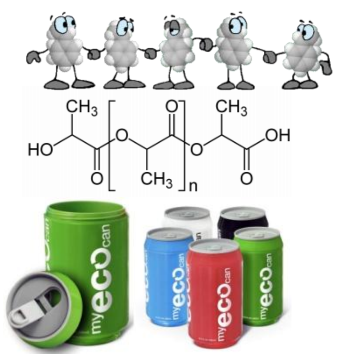
- 2-3 interested students
- Experience with C++
- High school organic chemistry definitely useful!
- IBM would provide some example inputs and outputs, and, of course, would be available to consult
- Goal: to return working code and test suite to OSRA developers for distribution under GNU public license

Example:

Lactic Acid



Poly (lactic Acid)



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