2007 Presentation

Biodegradable Plastics: Computational Modeling & Simulation of Starch Composites

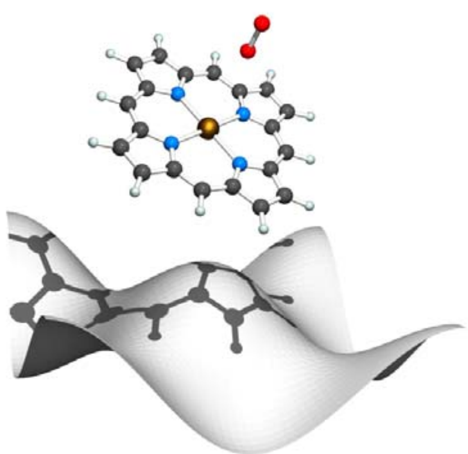
Presented By:

Sachin Joshi[1],Yuxin Zhuang[2],Yuming Zhang[2]

Dr. S.M. Sadjadi[1], Dr. A. M. Mebel[1]

1. Florida International University, Miami, USA

2. Computer Network Information Center (CNIC), Chinese Academy of Sciences, Beijing, China



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Overview

- Plastics
- Starch Composites
- Research Goals
- Computational Results
- Conclusions

Age of Plastics

Day to day uses - Packaging

Electrical appliances, automotive components

Aircraft & Aerospace industries

Biomedical Applications

Properties:

- High Strength
- Light weight
- Process-ability
- Chemical Stability

Plastics

Source of Plastics

Processing

Petroleum resources
Oil & Natural Gas

EXHAUSTIBLE !!!

DISPOSAL

Burning of Plastic wastes – Air Pollution

Dumping ???

Micro-organisms CANNOT
Break down the plastics into simple components

Non - biodegradable

Starch Composites

Natural Polymers

Starch & Cellulose – Natural polymers obtained from natural sources such as Corn, Rice, Grains etc.

They are broken down easily into simpler substances by micro-organisms

End Products: Water, Carbon dioxide, Inorganic compounds which acts as nutrients for plants

Starch – A potential candidate for biodegradable polymer

Starch Composites

STARCH

Advantages - Starch is found abundantly in plants and is Inexpensive

Bottlenecks - Starch is highly water-soluble and Weak in strength*.

How to improve the properties of starch?

Blend with HIGH STRENGTH polymer e.g. Poly-propylene carbonate (PPC)

Many strong polymers available to choose from…….

Compatibility Issues…....

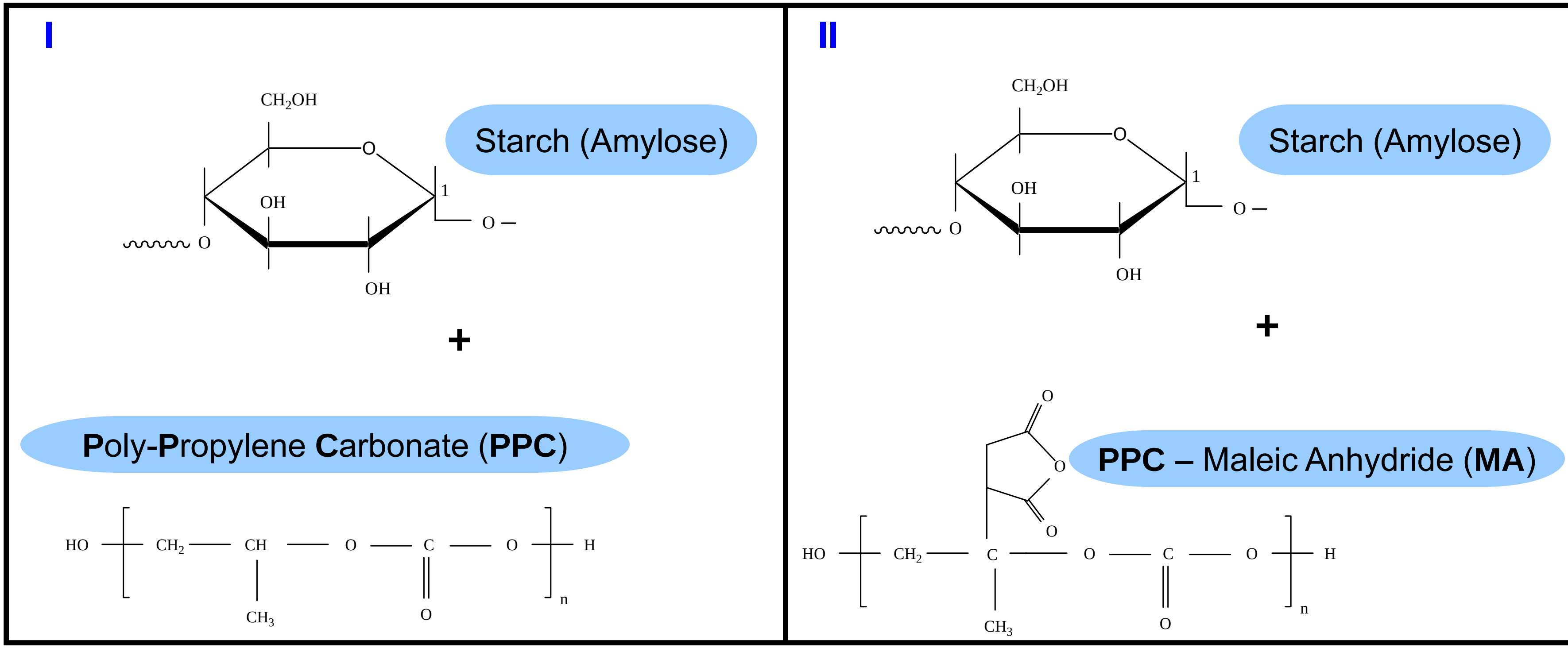
How to make a choice??

*Godbillot L, Dole P, Joly C, Roge B, MAthlouti M. Analysis of water binding in starch plasticized films. Food Chemistry; 96 (2006) 380-386

Research Goals

PROBLEM DESCRIPTION

Study 2 composites of Starch



ISSUES to be addressed:

- Which polymer more compatible with starch? Strong Composite

Research Goals

Computational Performance Analysis

- Perform 3 geometry optimization simulation runs using GAUSSIAN (molecular modeling software) which is installed on Chemistry Department cluster.

- Perform 3 single point energy simulation runs using MOLPRO (molecular modeling software) which is installed on GCB cluster in the following 2 phases:

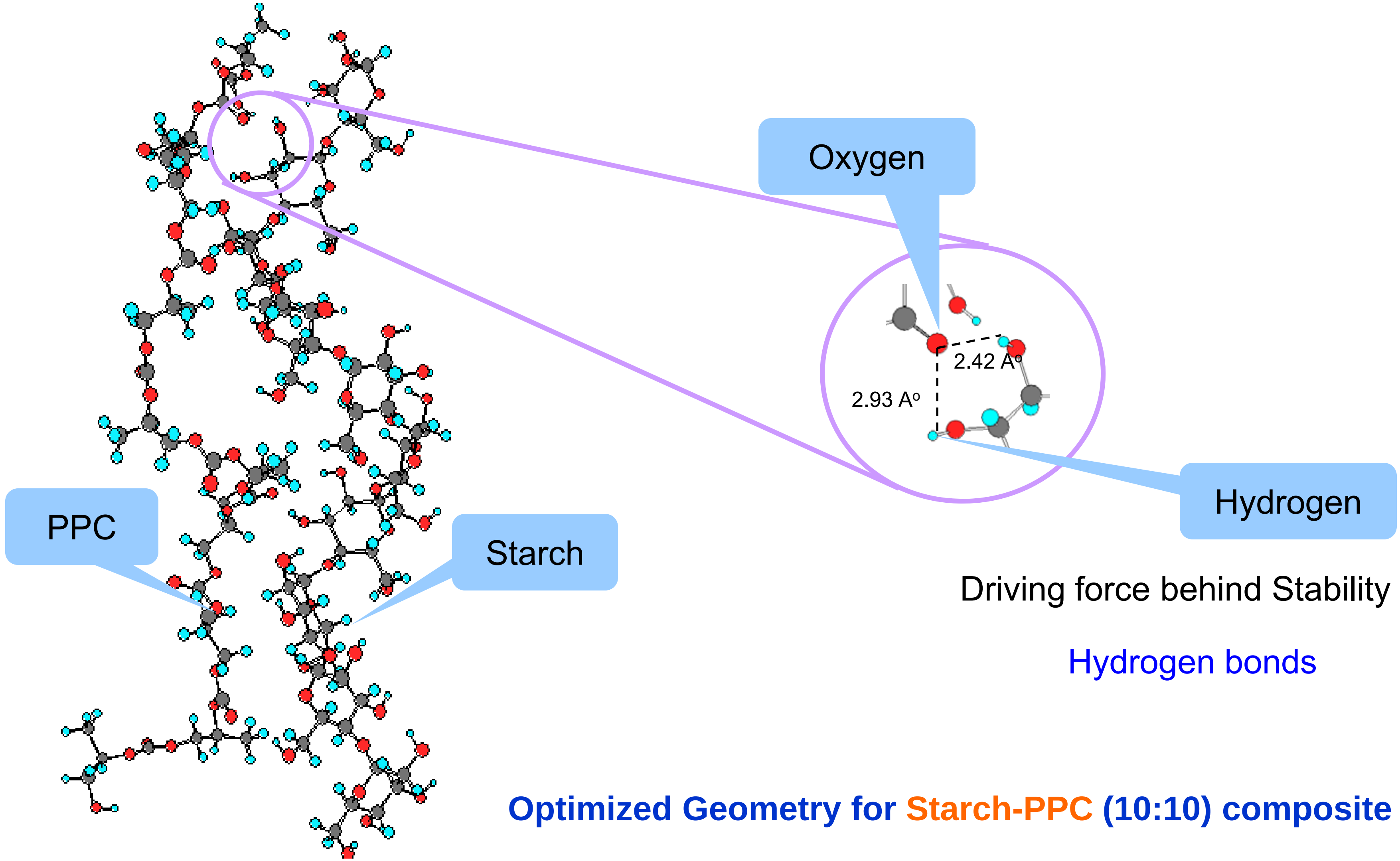
  (1) Single node computation.

  (2) Multi-node computation (parallel computation).

Computations run on GCB high performance cluster with
7 execution hosts
14 processors in total
SGE6.0 Scheduling

- Benchmarking computational results:
  Investigate how Parallel Computing will save computing time.
  - How job size effects a parallel job performance.
  - How a job Scheduling System influences the efficiency of a job.

Computational Results

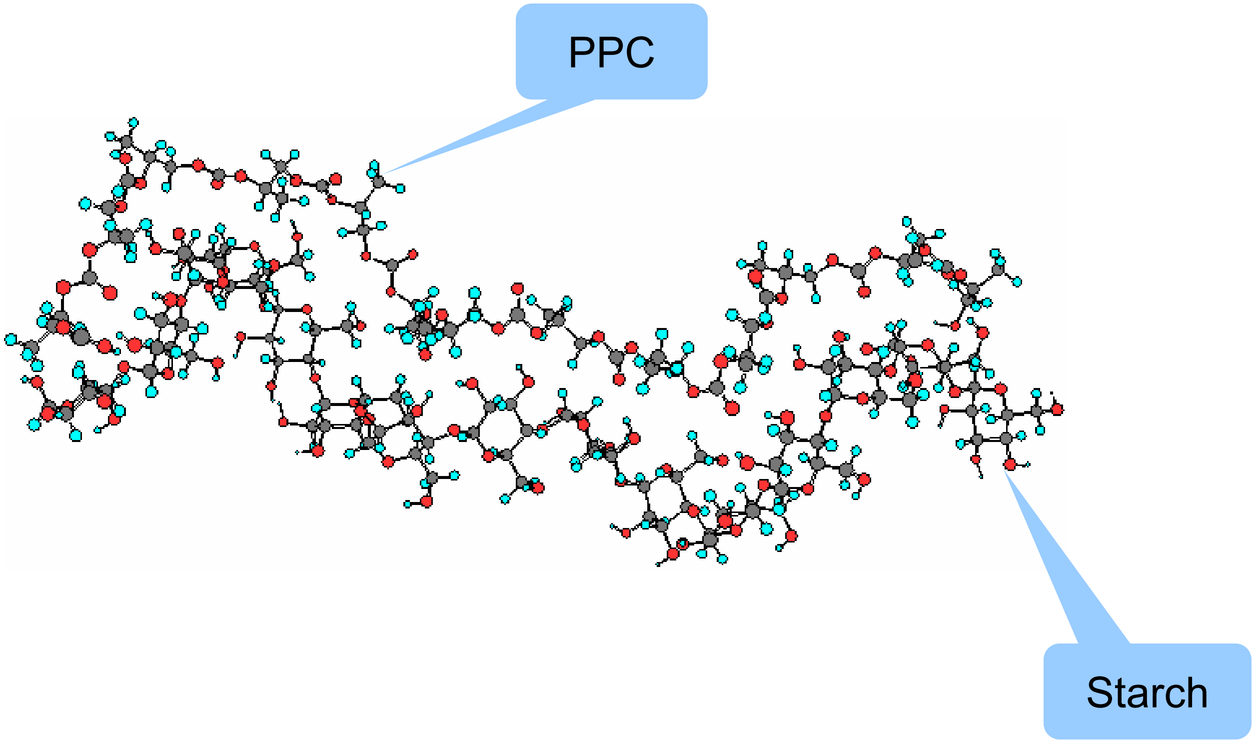


Driving force behind Stability ??

Hydrogen bonds

Optimized Geometry for Starch-PPC (10:10) composite

Optimized Geometry for Starch-PPC (15:15) composite



Computational Results

Stability of composites

Energy calculations show **Starch & PPC-MA** complexes are energetically stable

	Starch & PPC	Starch & PPC-MA	
Binding energy ΔE (kcal/mol)	-14.0	**-22.5**	**-18.3**

Reaction

Hydrogen bonds

Vibrational Frequency Analysis

Show more favorable interactions between **Starch and PPC-MA**

	Starch & PPC	Starch & PPC-MA
Change in C=O frequency (cm^{-1})	25	**42**

Computational Results

CPU times for 3 different jobs performed on MOLPRO with single-node computation

	1P	**1A**	**1A – 1P**
CPU time	29 mins:15 secs	2 hrs: 18 mins	1 day: 14 hrs

CPU times for a single job (1P) performed on MOLPRO with multi-node computation

# of Processors	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
CPU time (sec)	68	45	48	41	41	41	46	43	41	43	44	41	40	47

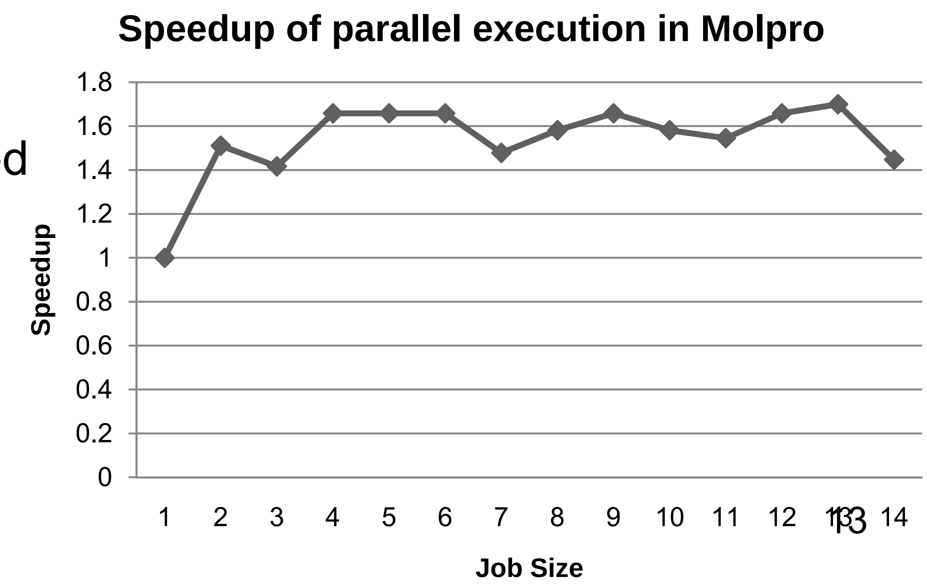
Effects of job size on parallel execution performance

- Parallel execution improves a job's performance by a non-linear speedup.
  - Speedup loss arises from
    a. I/O reads and writes of temporary data
    b. Communications in multi-node machines
    c. System overhead
    d. Parallelization overhead

Smaller job was selected.

With a bigger job – writing error occurred as tmp files were too large.

Small job – saved CPU time too small
large processors have to be allocated



Scheduling policy improves efficiency of parallel execution

- One can allocate priorities to the job which expects long running time

- Identify advanced scheduling policies
    I. Resource Reservation
    II. Backfilling

Conclusions

- Starch & PPC composite compared with Starch & PPC-MA
- Molecular modeling computations performed – GAUSSIAN & MOLPRO software
- Starch & PPC - MA composite more stable than Starch & PPC
- PPC-MA more compatible with Starch as compared to PPC
- Parallel execution in GCB cluster improves the job's performance by a non-linear speedup

Thank You