Using Parallel Computing in Drug Design

Richard A. Brown, St. Olaf
Elizabeth Shoop, Macalester College
Suzanne J. Matthews, West Point
Joel C. Adams, Calvin College
How do pharmaceutical companies design the medicines we use?
How medicines work

- Our DNA is like a book of recipes

- Instead of food, DNA contains the instructions for making proteins in our bodies
How medicines work

• A protein’s shape determines the function it performs in a person’s body

• To design a drug, we can find ligands (new pieces) to change a protein’s shape
How medicines work
Strategy for drug design software

1. Generate ligands to try for particular protein
   – Some ligands will fit, some won’t

2. Compute a score for each ligand that simulates how well it will:
   – fit that protein; and
   – produce a desired shape change

3. Identify the highest scoring ligands for actual synthesis (production) and testing
Drug design exemplar code

A program *structured like* drug design software

1. **Generate ligands** to try for particular protein
   – Random character *strings* of random lengths

2. **Compute a score for each ligand**
   – Compare for **maximum match**
     with string representing a protein
   – Insertions and deletions allowed

3. Identify the **highest scoring ligands**
Drug design exemplar code

A program *structured like* drug design software

1. Generate ligands to try for particular protein
   - **Fast**

2. Compute a *score* for each ligand
   - Takes a long time
   - **Parallelize** by using *multiple computation threads* for different ligands

3. Identify the *highest scoring* ligands
   - **Fast** – just sort and find maximum
Drug design exemplar code

Command-line arguments:

./drugdesign-static threads maxlen count

• **threads** is number of simultaneous threads
• **maxlen** is *maximum* length of a ligand
  – *Each ligand* has random length up to this max
• **count** is number of ligands to score