Drinking from a firehose: Solving data analysis challenges posed by the Anton supercomputer

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**Biomolecular Timescales (seconds)**

- **fs** – fastest motions of hydrogen bond (one MD step = 2 fs)
- **μs** – basic biochemical sub-steps (a half-billion steps)
- **ms** - this is where biological processes start to get interesting (a half-trillion steps: years of simulation of a modern general-purpose supercomputer or cluster)

Adapted from Suits (IBM), originally from Chan & Dill (1993)
Why Molecular Dynamics (MD) is hard...

Bonded

Non Bonded: Van der Waals, Near Electrostatics

Non Bonded: Far Electrostatics

\[
E = \sum_{\text{bonds}} k_b (r - r_0)^2 + \sum_{\text{angles}} k_\theta (\theta - \theta_0)^2 + \sum_{\text{torsions}} A[1 + \cos(n\tau - \varphi)] + \sum_i \sum_{j>i} \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6} + \sum_i \sum_{j>i} \frac{q_i q_j}{r_{ij}}
\]
Time required for one-millisecond simulation of a small protein

<table>
<thead>
<tr>
<th>Machine</th>
<th>Time required</th>
</tr>
</thead>
<tbody>
<tr>
<td>General-purpose supercomputer</td>
<td>2123 days (5.8 years)</td>
</tr>
<tr>
<td>Top-end 2019 GPU</td>
<td>806 days (2.2 years)</td>
</tr>
<tr>
<td>Anton 1 (2008)</td>
<td>55 days</td>
</tr>
<tr>
<td>Anton 2 (2013)</td>
<td>12 days</td>
</tr>
</tbody>
</table>

Joint AMBER-CHARMM benchmark of dihydrofolate reductase DHFR (23,558 atoms, 62 Å cube, $2.5 \times 10^{-15}$ s time step)
512-node Anton Performance

![Graph showing performance vs number of atoms for different Anton configurations]

- Anton 2 water box
- Anton 2 protein
- Anton 1 water box
- Anton 1 protein

Performance (μs/day)

Number of atoms

D E Shaw Research
Our Answer: Anton: A family of specialized supercomputers for MD simulation
Roadmap

Anton 1 ASIC
Bringup
Production

Anton 2 ASIC
Bringup
Production

Anton 3 ASIC
Anton 2 Architecture: 3D Torus of Directly Interconnected ASICs (nodes)
Flexible Subsystem Tile (Flex)

- Dispatch Unit
- 256 KB SRAM
- Network Interface
- Geometry Core
- Geometry Core
- Geometry Core
- Geometry Core
High-Throughput Interaction Subsystem (HTIS)
Cool and Connected

Board

Rack

Air flow
Anton 2: In production since 2014
Anton 2 produces ~100MB/s of output data

× 86,400 seconds/day
× 365 days/year....

= 3.2 PB/year

We archive all of it.

Now what...
Track everything!

- Database with metadata about every Anton simulation
- Every simulation has a unique, permanent numeric id
- Input and output permanently archived
- Accessible via virtual filesystem (TreasureMap)
Reproducibility is essential

- Scientific
- Engineering
Scientific reproducibility: Dynamics
Reversible folding of 12 proteins to atomic resolution

Engineering reproducibility: hardware

- Fixed point
  - Give up dynamic range for precision
  - Overflows: Ignore (saturation) or Halt!
  - Bitwise reproducibility enormously easier
  - Less area than comparable floating point
  - Much less design effort

- Network predictability
  - Communication patterns
  - In-network reduction
Engineering Software reproducibility

• “garden” of all software versions stored in different paths
• Expose explicit version to end-users
  – No default
• Versions are U.N.F (e.g. 2.7.31)
  – U = major change to User input format
    • Semantics or default assumptions changed
  – N = numerics change
  – F = fix or new features, bitwise reproducible
• Versioning must be a transitive closure
• Cannot rely on OS/distro-supplied math, compilers or interpreters
The result: Reproducible research

- Our researchers conduct long-timescale projects, spanning years of runs
  - usually staying with a single U.N.* series (we do backport some fixes)
- Reduced output and checkpoint rates
  - Can “zoom” by re-running parts of a trajectory
- Trust but verify:
  - 1-5% of our machine time every day is for automated re-runs of parts of jobs
  - Every mismatch automatically opens a ticket: is it a software bug, hardware error.
Biomolecular Research using Anton

- Longest all-atom, explicit solvent MD runs before Anton 1 were about 10 microseconds.
- Anton 1 *routinely* simulated biomolecules to $O(100)$ microseconds, Anton 2 easily reaches milliseconds (and on larger molecules), allowing us to observe and understand:
  - Protein folding
  - Changes in protein conformation (and how conformations relate to function)
  - How a drug binds to a protein
  - How to find new targets for drug discovery
0.0 μs

P. Maragakis et al, Unpublished.
Questions?