Electrostatics of nanosystems: Application to microtubules and the ribosome

Nathan A. Baker, David Sept, Simpson Joseph, Michael J. Holst, J. Andrew McCammon

Presentation by Alex Heitman
A faster more efficient way to calculate the Poisson Boltzmann equation (used to solve the electrostatic potential)

PBE is a complex non-linear second order partial differential equation

utilize multiple processors and parallel computing

Parallel Focusing = Bank Holst + Electrostatic Focusing
Motivation

- Molecular Dynamics – modeling molecular interaction via the laws of physics and chemistry
- Important in understanding protein folding could help understand many phenomena including diseases
- Each molecular configuration change results in a new potential which must be solved again
- Clearly PBE is a key computationally expensive step which must be solved repeatedly
PBE - Solving Complex PDE's

- Computationally expensive
- Even the linearized PBE (LPBE) presents a daunting task
- Many methods (finite difference, finite element, boundary element, etc.)
- Finite Difference – covered by RC
Finite Element Method

- Splits the domain into subdomains – usually triangular mesh pattern
- Creates a basis of equations
- Approximates the solution equation in terms of the basis
- FEMLAB
Finite Element vs. Finite Difference

- Key difference: FEM approximates the solution, FDM approximates the differential equation.
- For PBE/LPBE it seems that FDM is preferred.
- FEM is more adept for parallel computing.
- FEM good for irregular domains (complex geometries, varying precision).
- FDM takes up a lot of memory.
- Overall the choice seems to be problem dependent.
Bank Holst Algorithm

- Multiprocessor usage with minimal inter-processor communication
- A rough global solution using FEM
- Each Processor given a subdomain based upon equal error distribution
- Adaptive refinement of the subdomain by enriching the basis set of that region, reevaluation with FEM
Electrostatic “focusing”

- Finite difference method
- Solves for the entire domain using a coarse grid
- Uses rough solution to generate boundary conditions for the target subdomain
- Uses a tighter grid over subdomain with the given boundary conditions
Parallel Focusing

1) solve the coarse solution over the global domain \((BH, f)\)

2) subdivides the global domain into \(P\) subdomains each assigned to individual processor \((BH)\)

3) locally solved with FDM using boundary conditions from initial sol’n \((f)\)

4) master processor collects local sol’ns and gives a refined global sol’n
Tubulin: Parallel Focusing at work

- Tubulin in the microtubules of the cytoskeleton
- 1.25 million atoms
- Using parallel focusing solution reached in one hour
- Similar resolution required 350 times the memory and time
- Revealed the overall negative potential of tubulin with smaller pockets of + potential
- Parallel focusing – linear increase in time efficiency per processor
Conclusion

- With shorter computing time, parallel sol’ns makes the solving of large biomolecular systems less daunting.
- Interesting features near drug binding sites of microtubules revealed through parallel focusing.