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

Subject= Parallel Focusing

- A faster more efficient way to calculate the Poisson Boltzmann equation (used the 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 approx's the differential eq'n
- 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