Parallel Implementation of multipole-based Poisson-Boltzmann solver

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CS 267 Project

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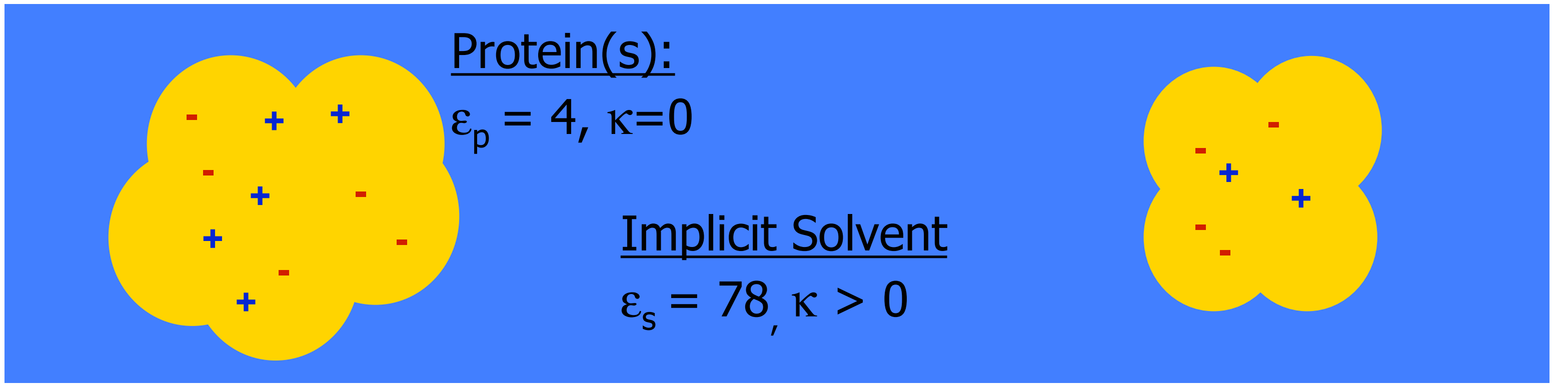
UCSF & UCB joint graduate group in BIOENGINEERING

Simulation Overview


Protein(s):
$\varepsilon_p = 4$, $\kappa=0$
Implicit Solvent
$\varepsilon_s = 78$, $\kappa > 0$

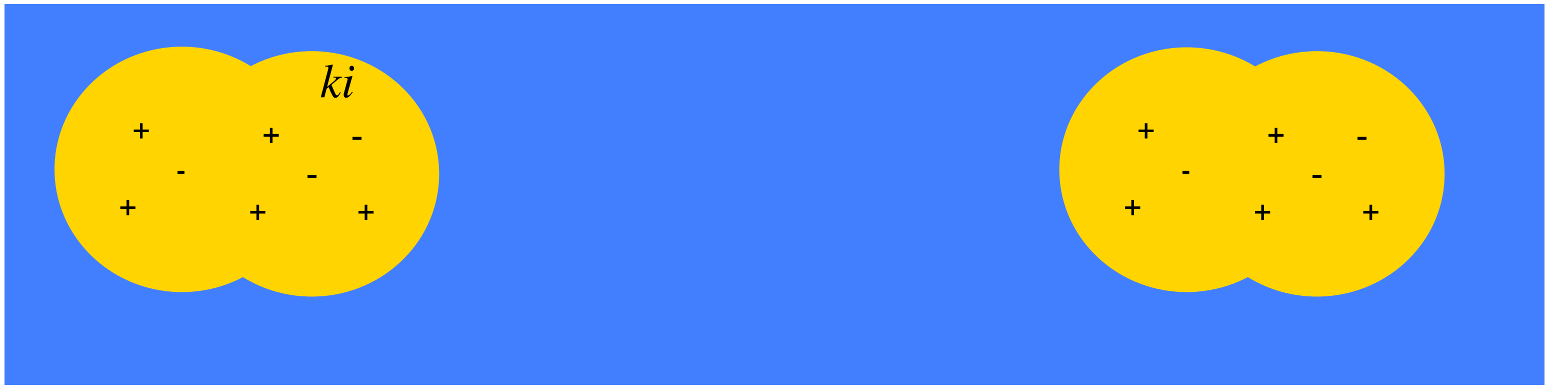
1. **Initialize system**
2. **Calculate forces**
   - Solve linearized Poisson Boltzmann Equation (LPBE)

$$\boxed{-\nabla\left[\varepsilon(\mathbf{r})\nabla\Phi(\mathbf{r})\right]+\kappa^2\Phi(\mathbf{r})=\rho_{fixed}(\mathbf{r})}$$

3. **Propagate Molecules**
   - Brownian Dynamics using forces from (2)

4. **Repeat** 2-3 until criteria is met

Solving LPBE with Multipole Method



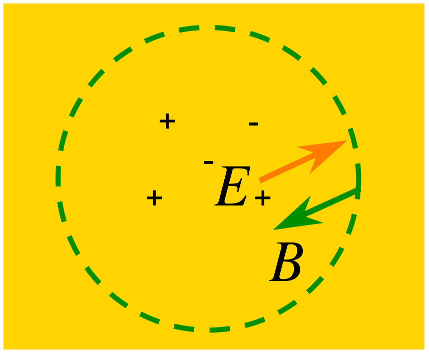
Each molecule is represented as a collection of spheres.

For each sphere *ki*:

1. Calculate surface charge multipole S_{nm}
   (i) Express Φ_{in} and Φ_{out} in terms of multipoles
   (ii) Setting up boundary equations.
   (iii) Solve for S_{nm}
2. Update contribution from S_{nm} to other spheres
3. Repeat for all spheres until convergence criteria is reached

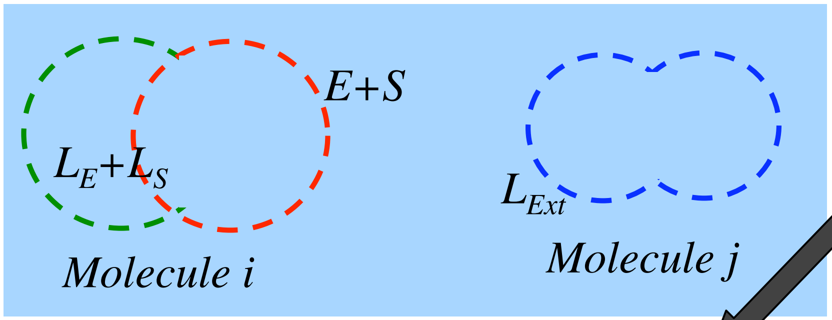
(i) Potential Equations (in terms of multipoles)

Inside sphere ki:



$$\Phi_{in}^{(ki)}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{E_{Fixed\,nm}^{(ki)}}{r^{n+1}} + r^n B_{nm}^{(ki)} \right) Y_{nm}(\theta,\phi)$$

Outside sphere ki:



Goal: Solve for unknown S

$$\Phi_{out}^{(ki)}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{(E_{Fixed} + S)_{nm}^{(ki)}}{r^{n+1}} + (L_s + L_E + L_{Ext})_{nm}^{(ki)} r^n \right) Y_{nm}(\theta,\phi)$$

(ii) Boundary conditions

On sphere *ki's* surface *(a,θ,ϕ)*:

$$\boxed{\Phi_{in}(\mathbf{r})\Big|_{Surface_{ki}} = \Phi_{out}(\mathbf{r})\Big|_{Surface_{ki}}}$$

$$\boxed{\varepsilon_{in}\frac{d\Phi_{in}(\mathbf{r})}{dn}\Bigg|_{Surface,ki} = \varepsilon_{out}(\theta,\varphi)\frac{d\Phi_{out}(\mathbf{r})}{dn}\Bigg|_{Surface,ki}}$$

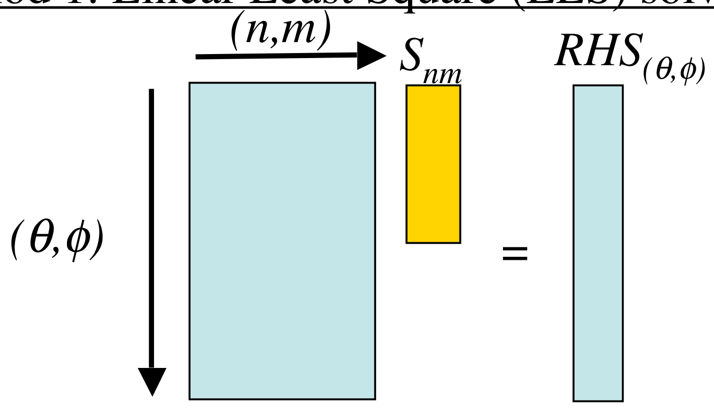
$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left[n\varepsilon_p + (n+1)\varepsilon_{out}(\theta,\phi)\right]S_{nm}^{(ki)}Y_{nm}(\theta,\phi)$$

$$= \left(\varepsilon_{out}(\theta,\phi)-\varepsilon_p\right)\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\Big\{\underbrace{-(n+1)E_{nm}^{(ki)} + an\left(L_s + L_E + L_{Ext}\right)_{nm}^{(ki)}}_{X_{nm}}\Big\}Y_{nm}(\theta,\phi) \qquad (*)$$

(iii) Solving Boundary Equation (*) for S_{nm}

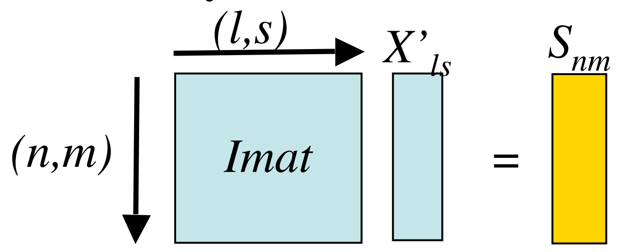
Represent (*) as linear system of equations, solve S_{nm} up to p poles:

Method 1: Linear Least Square (LLS) solvers



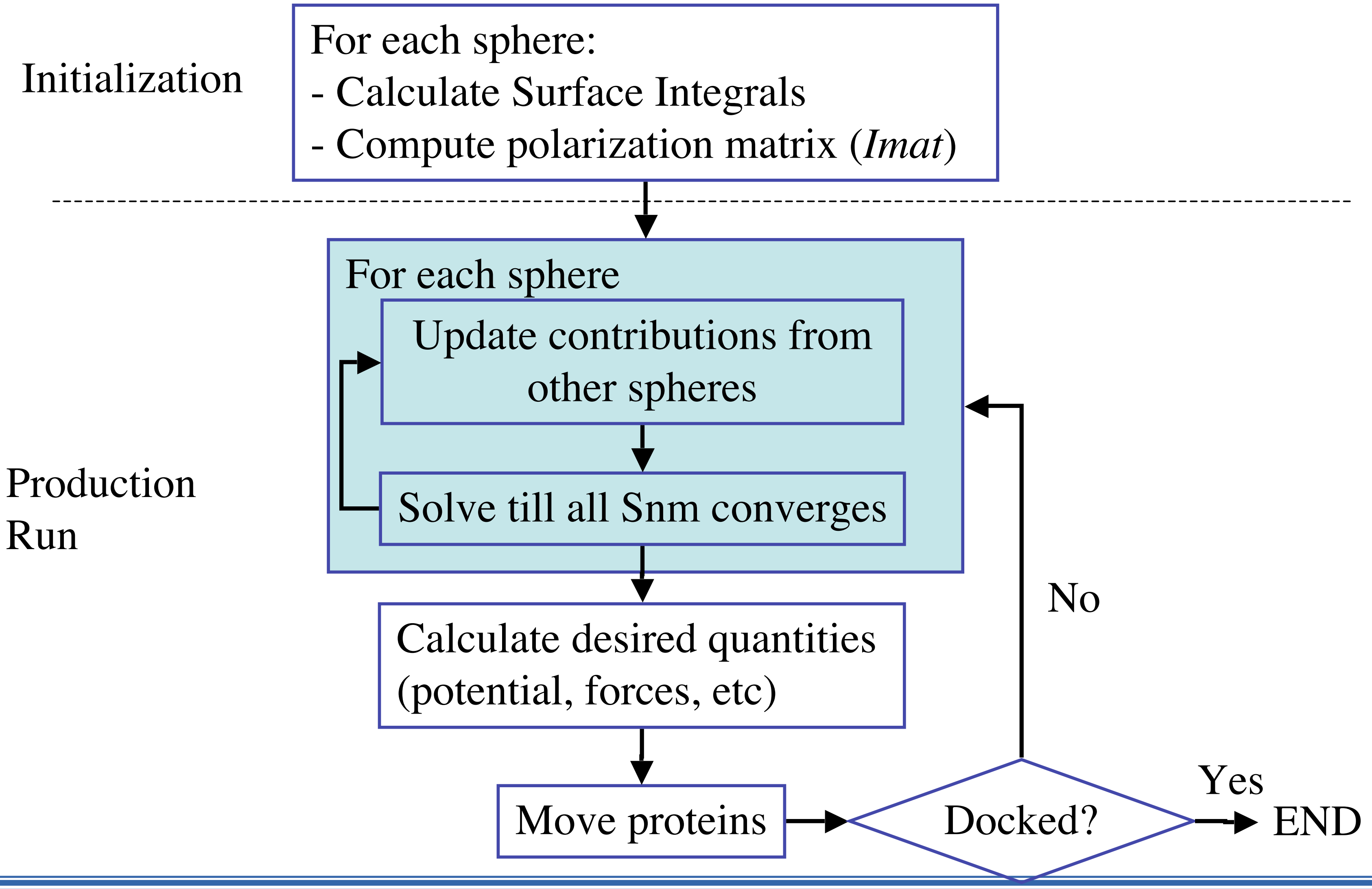
Requires LLS solver
-> Inefficient!
For p=60: ~ 10min per solution

Method 2: Analytical, iterative method using orthonormality property of SH



Matrix-Vector Multiply
-> Fast
For p=60:
Initial matrix prep ~ 14min per sphere
Subsequent solution ~ 0.4s

Simulation Algorithm (Serial)



Initialization
For each sphere:
- Calculate Surface Integrals
- Compute polarization matrix (*Imat*)
Production Run
For each sphere
Update contributions from other spheres
Solve till all Snm converges
Calculate desired quantities (potential, forces, etc)
Move proteins
Docked?
No
Yes
END

Parallization Strategy

Parallelization at sphere level

- solve Snm for each sphere separately and share updated values with other spheres
- Jacobi iteration vs. Gauss-Seidel iterations

1) Shared Memory Only Model

- adequate for small systems (< 10 spheres)

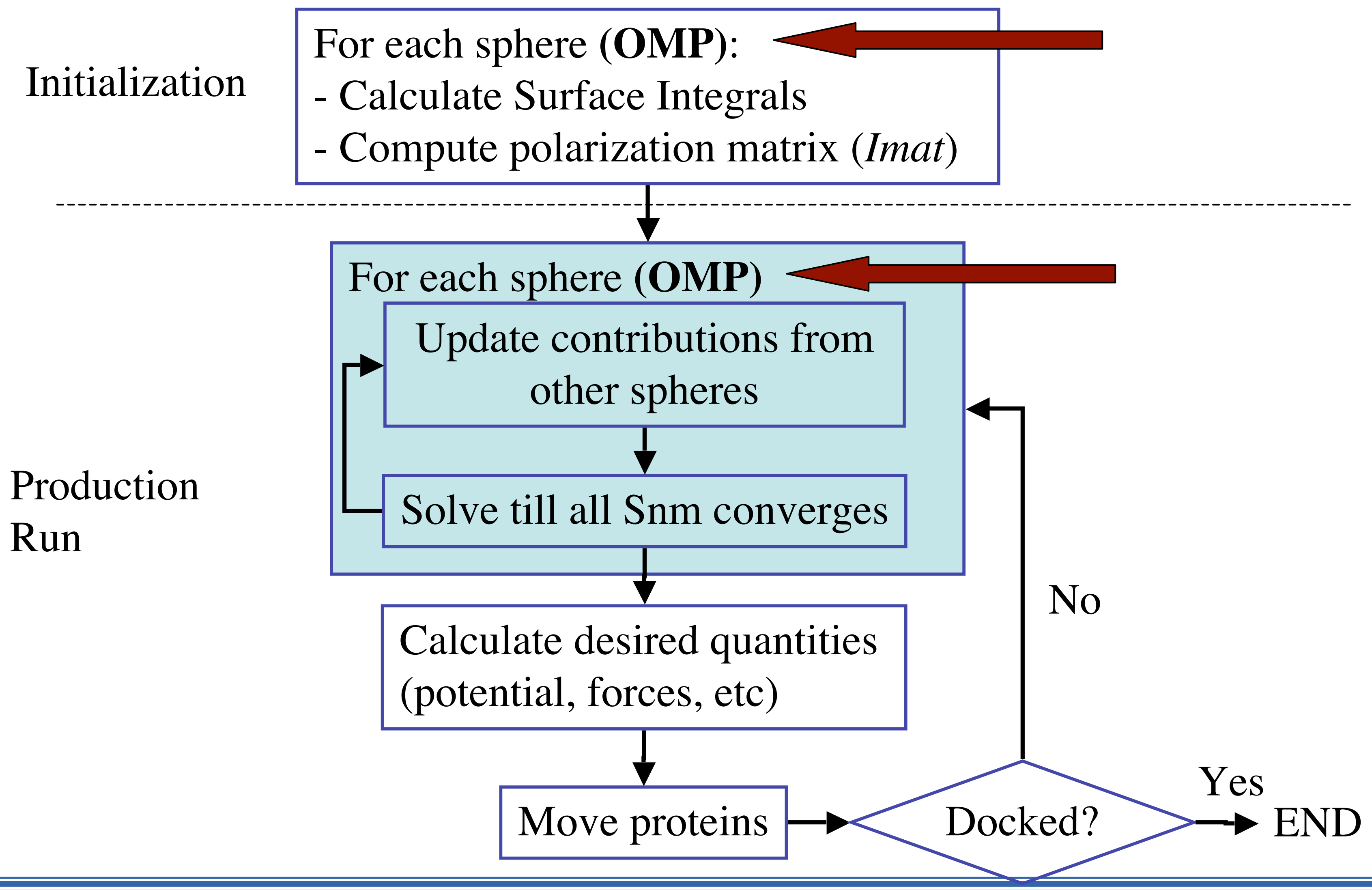
- Using OpenMP
- Easy implementation within c++ object-oriented code

2) Hybrid Model

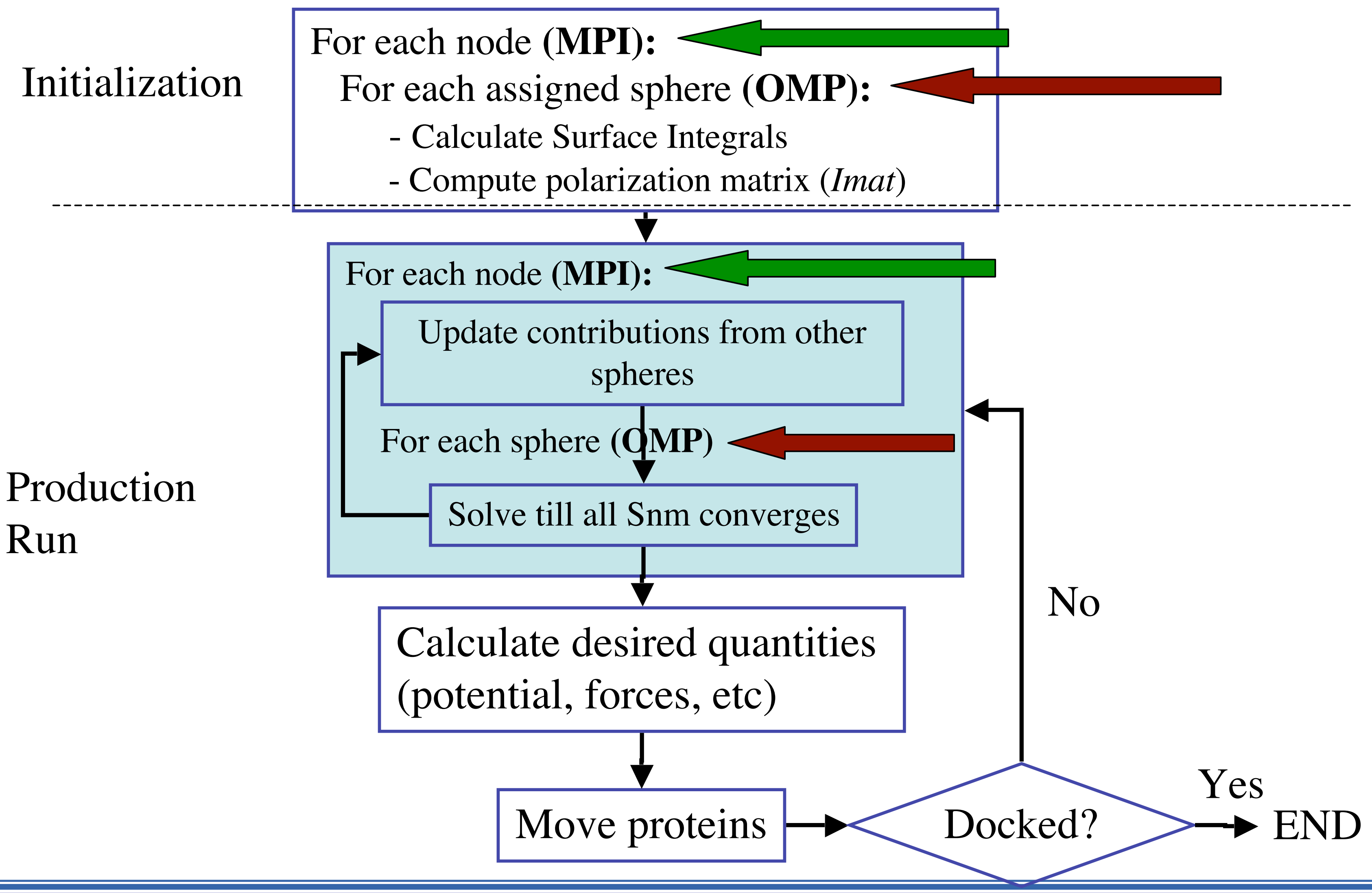
- required for larger scale systems (> 10 spheres)

- Intra-node: shared memory using OpenMP
- Inter-node: distributed memory using MPI
- C++ objects need to be packed/unpacked for MPI communications

Simulation Algorithm (Shared Memory)

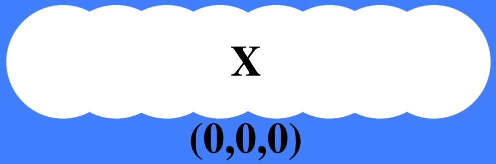

Initialization
For each sphere (OMP):
- Calculate Surface Integrals
- Compute polarization matrix (Imat)
For each sphere (OMP)
Update contributions from other spheres
Solve till all Snm converges
Production Run
Calculate desired quantities (potential, forces, etc)
Move proteins
Docked?
No
Yes
END

Simulation Algorithm (Hybrid)

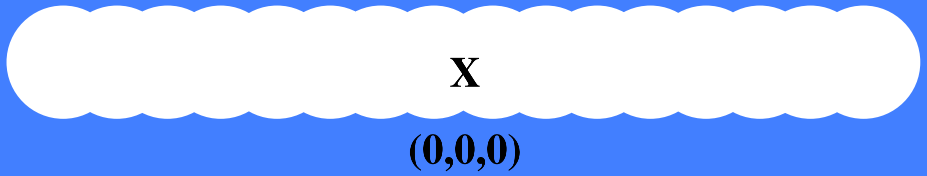

Initialization
For each node (MPI):
For each assigned sphere (OMP):
- Calculate Surface Integrals
- Compute polarization matrix (*Imat*)
Production Run
For each node (MPI):
Update contributions from other spheres
For each sphere (OMP)
Solve till all Snm converges
Calculate desired quantities (potential, forces, etc)
Move proteins
Docked?
No
Yes
END

Test cases for Timing

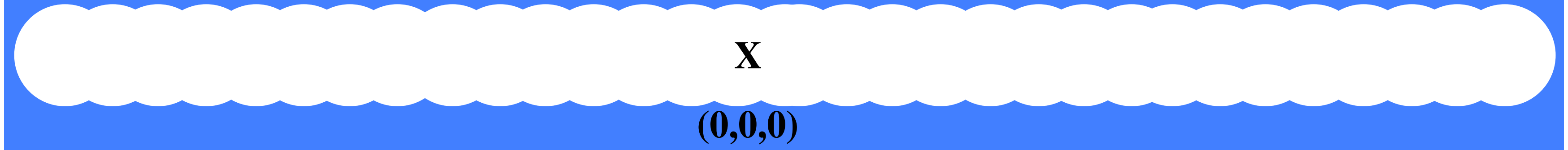
A) 8 overlapping spheres



B) 16 overlapping spheres

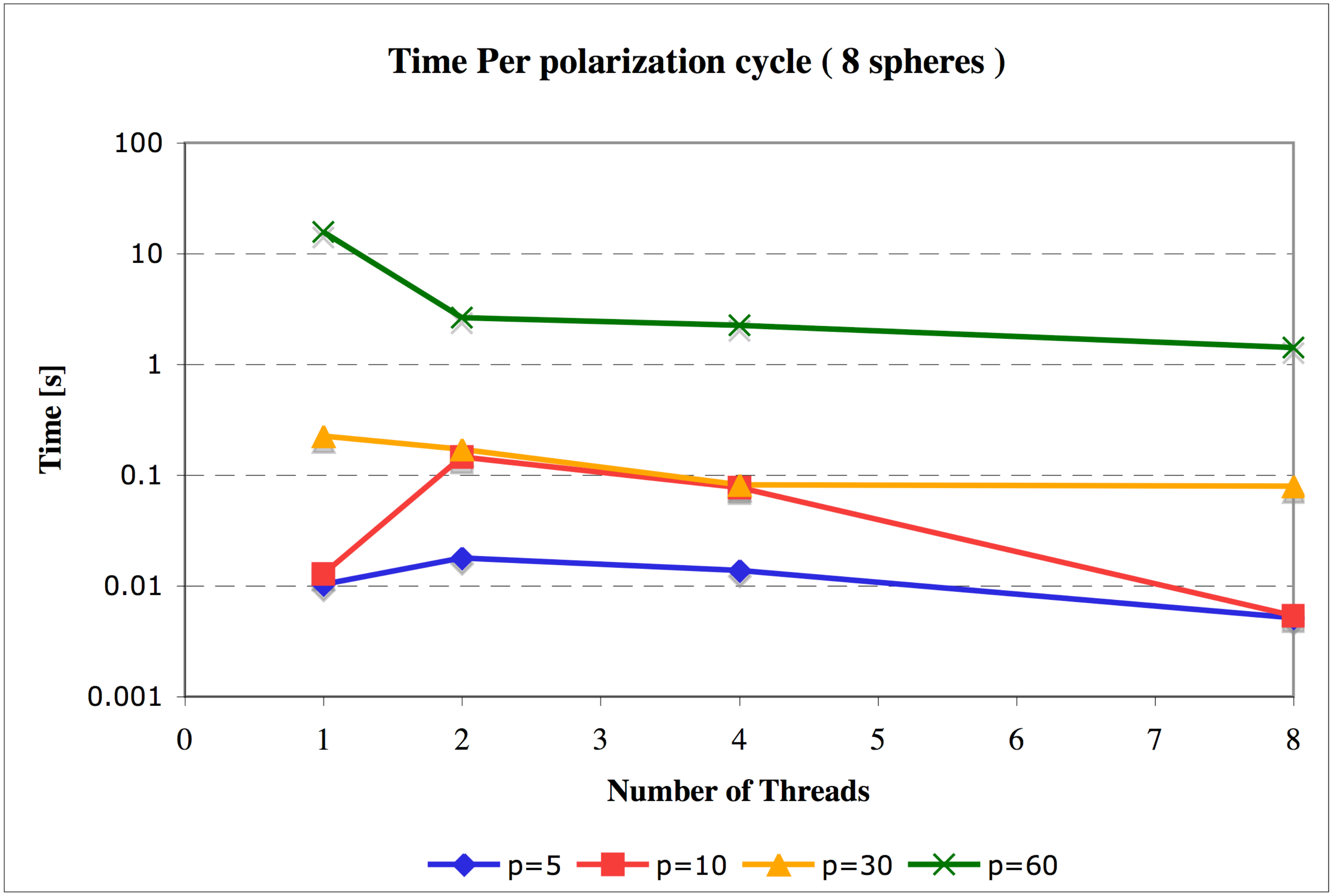


C) 32 overlapping spheres



- Different no. of poles used (p = 5, 10, 30, 60)
- Different no. of threads used (t = 1, 2, 4, 8)

Preliminary Timing Results (Shared Memory)


Time Per polarization cycle (8 spheres)
Time [s]
Number of Threads
p=5
p=10
p=30
p=60