Electrostatics & the Laplace equation

Outline

- Topic motivation:
  - I would like to bring in more elements from other courses in the Engineering Physics program
    - Bring in elements of course EI1320 on electromagnetism
- Contents and assignments from chapter 10 in the book
- Short introduction on electrostatics and the Laplace equation
- Some generalizations (not for assignments)
- Assignments

Static charges

- The electric Field **E** at point **r** due to charges $q_1, q_2, \ldots, q_N$

$$\mathbf{E}(\mathbf{r}) = K \sum_{i}^{N} \frac{q_i}{|\mathbf{r} - \mathbf{r}_i|^3} (\mathbf{r} - \mathbf{r}_i)$$

$$K = \frac{1}{4\pi\epsilon_0} \approx 9.0 \times 10^9 \,\mathrm{N \cdot m^2/C^2}$$

- K is inconvenient, often absorbed into the charges (Gaussian units)

Electric potential

It often is easier to analyze the behavior of a system using energy rather than force concepts. We define the electric potential $V(\mathbf{r})$ by the relation

$$V(\mathbf{r}_2) - V(\mathbf{r}_1) = -\int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{E} \cdot d\mathbf{r}, \tag{10.6}$$

or

$$\mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r}). \tag{10.7}$$

Only differences in the potential between two points have physical significance. The gradient operator ∇ is given in Cartesian coordinates by

$$\nabla = \frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial z}\hat{\mathbf{z}}, \tag{10.8}$$

where the vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are unit vectors along the x, y, and z axes respectively. If V depends only on the magnitude of $\mathbf{r}$, then (10.7) becomes $E(r) = -dV(r)/dr$. Recall that $V(r)$ for a point charge q relative to a zero potential at infinity is given by

$$V(r) = \frac{q}{r}. \qquad \text{(Gaussian units)} \tag{10.9}$$

Boundary value problems

- The Laplace equation:

$$\nabla^2 V(x,y,z) \equiv \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0$$

- Simplest example of elliptic partial differential equation
- Used in:
  - Electromagnetism
  - Astronomy
  - Fluid Dynamics
- Relaxation of this potential is closely related to diffusion (see e.g. chapter 7 of the course book)

Solving the Laplace equation

- The Laplace equation:

$$\nabla^2 V(x,y,z) \equiv \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0$$

- Finite difference, remarkably simple:

$$\begin{aligned} V(x,y) \approx \frac{1}{4}[&V(x+\Delta x, y) + V(x-\Delta x, y) \\ &+ V(x, y+\Delta y) + V(x, y-\Delta y)] \end{aligned}$$

- From Taylor expansion:

$$V(x+\Delta x, y) = V(x,y) + \Delta x \frac{\partial V(x,y)}{\partial x} + \frac{1}{2}(\Delta x)^2 \frac{\partial^2 V(x,y)}{\partial x^2} + \ldots$$

$$V(x, y+\Delta y) = V(x,y) + \Delta y \frac{\partial V(x,y)}{\partial y} + \frac{1}{2}(\Delta y)^2 \frac{\partial^2 V(x,y)}{\partial y^2} + \ldots$$

The Poisson equation

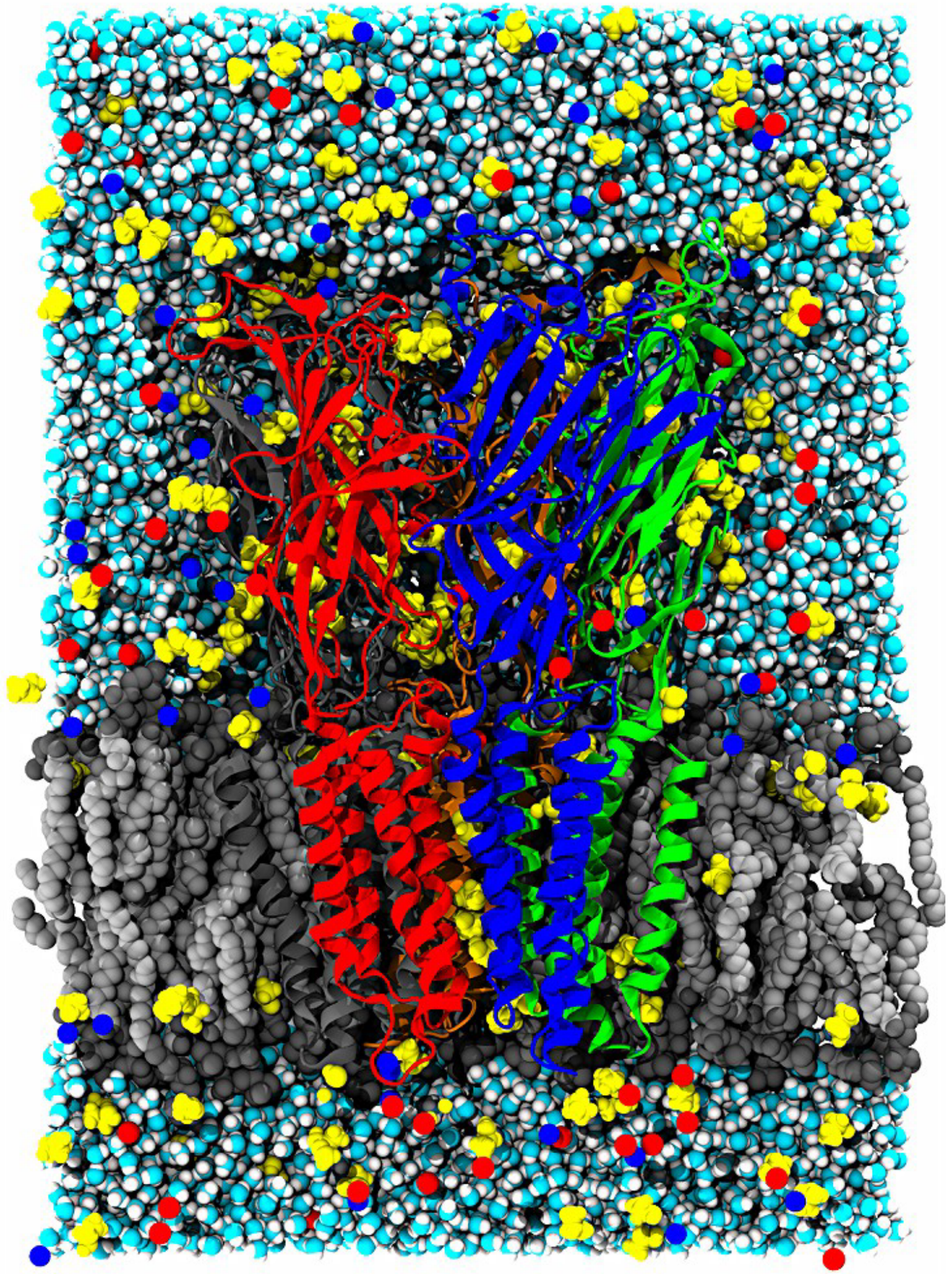
- Laplace's equation holds only in charge free regions
- With a charge density ρ(x,y,z) use the Poisson equation:

$$\nabla^2 V(\mathbf{r}) = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -4\pi\rho(\mathbf{r})$$

Poisson equation in Molecular Dynamics

Need to get the electrostatic forces between (partial) charges on atoms

We use Fast Fourier Transforms (FFT), solving Poisson's equation is a multiplication in Fourier space



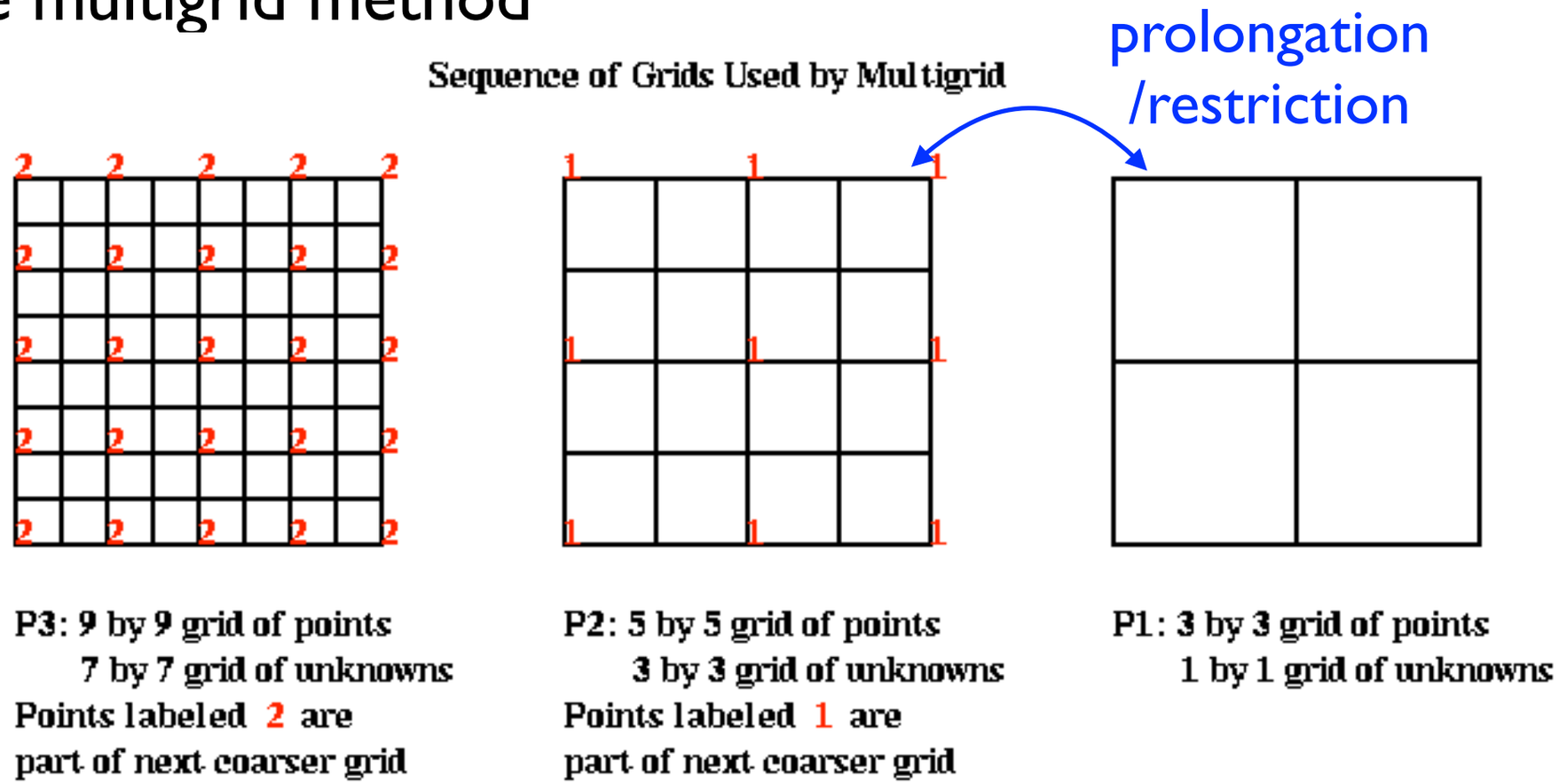
Fast methods for large Poisson problems

- The interaction kernel 1/r has decreasing gradient:
  - details at small length scales matter less over large distance
  - Fast methods make use of this
    - On grid: Multi-grid method O(N)
    - Off grid: Fast multipole method O(N)

The multigrid method

- With the simple finite difference method relaxation on long length scales is very slow: iterations $\propto$ grid size

- This can be improved significantly by using what is called the multigrid method



Random Walk Solution of Laplace's Equation

1. Begin at a point (x, y) where the value of the potential is desired, and take a step in a random direction.

2. Continue taking steps until the walker reaches the surface. Record $V_b(i)$, the potential at the boundary site i. A typical walk is shown in Figure 10.4.

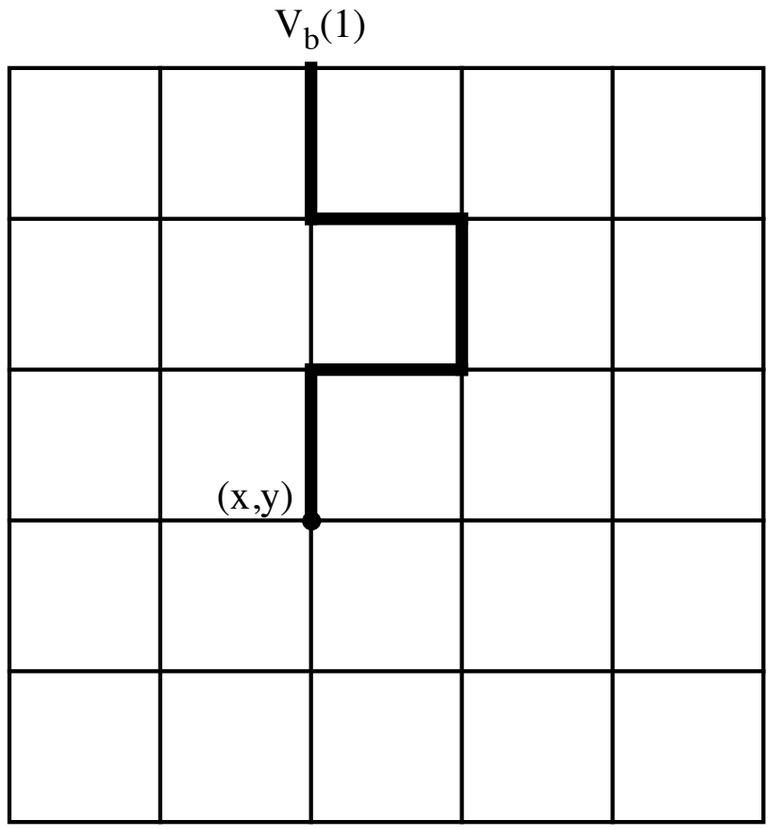
3. Repeat steps (1) and (2) n times and sum the potential found at the surface each time.

4. The value of the potential at the point (x, y) is estimated by

$$V(x, y) = \frac{1}{n} \sum_{i=1}^{n} V_b(i) \tag{10.25}$$

where n is the total number of random walkers.

A random walk on a 6 Å~ 6 grid starting at the point (x, y) = (3, 3), ending at the boundary site $V_b(3, 6)$ where the potential is recorded.



Green's function

Given a linear differential operator $\mathcal{L} = \mathcal{L}(x)$ acting on the collection of distributions over a subset Ω of some Euclidean space $\mathbb{R}^n$, a Green's function $G = G(x, s)$ at the point $s \in \Omega$ corresponding to $\mathcal{L}$ is any solution of

$$\mathcal{L}G(x, s) = \delta(x - s)$$

where δ denotes the delta function. By multiplying the above identity by a function $f(s)$ and integrating with respect to s yields $\int \mathcal{L}G(x, s) f(s)\, ds = \int \delta(x - s) f(s)\, ds.$

The right-hand side reduces merely to $f(x)$. Because $\mathcal{L}$ is a linear operator acting only on x and not on s, the left-hand side can be rewritten as

$$\mathcal{L}\left(\int G(x, s) f(s)\, ds\right).$$

Particularly useful when solving for $u = u(x)$ in differential equations of the form $\mathcal{L}u(x) = f(x)$,

where the above arithmetic confirms that $\mathcal{L}u(x) = \mathcal{L}\left(\int G(x, s) f(s)\, ds\right)$

and whereby it follows that u has the specific integral form $u(x) = \int G(x, s) f(s)\, ds.$

Green's function from random walks

The disadvantage of the random walk method is that it requires many walkers to obtain a good estimate of the potential at each site. However, if the potential is needed at only a small number of sites, then the random walk method might be more appropriate than the relaxation method, which requires the potential to be computed at all points within the region. Another case where the random walk method is appropriate is when the geometry of the boundary is fixed, but the potential in the interior for a variety of different boundary potentials is needed. In this case the quantity of interest is $G(x, y, x_b, y_b)$, the number of times that a walker from the point (x, y) lands at the boundary (x_b, y_b). The random walk algorithm is equivalent to the relation

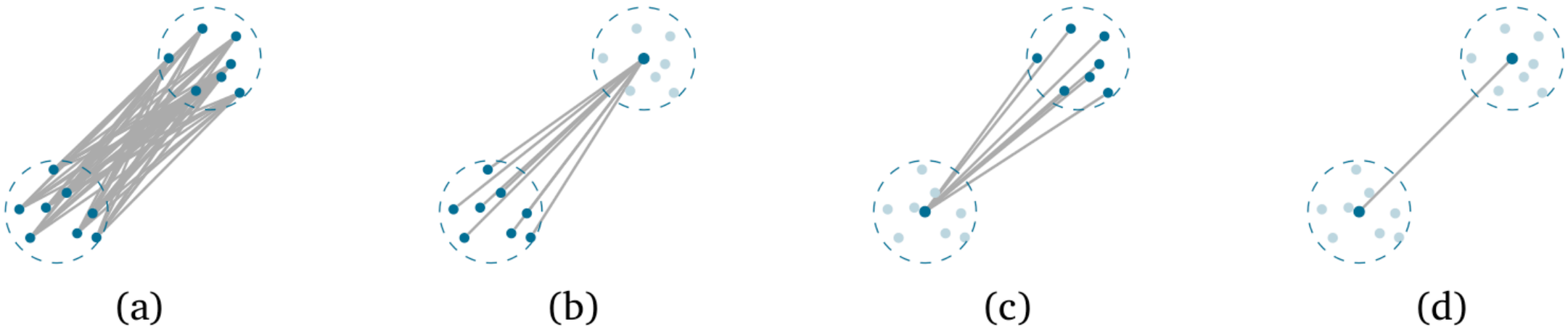
$$V(x,y) = \frac{1}{n} \sum_{x_b, y_b} G(x, y, x_b, y_b) V(x_b, y_b) \tag{10.26}$$

where the sum is over all sites on the boundary. We can use the same function G for different distributions of the potential on a given boundary. G is an example of a Green's function, a function that you will encounter in advanced treatments of electrodynamics and quantum mechanics (cf. Section 16.9). Of course, if we change the geometry of the boundary, we have to recompute the function G.

Advanced methods for electrostatics

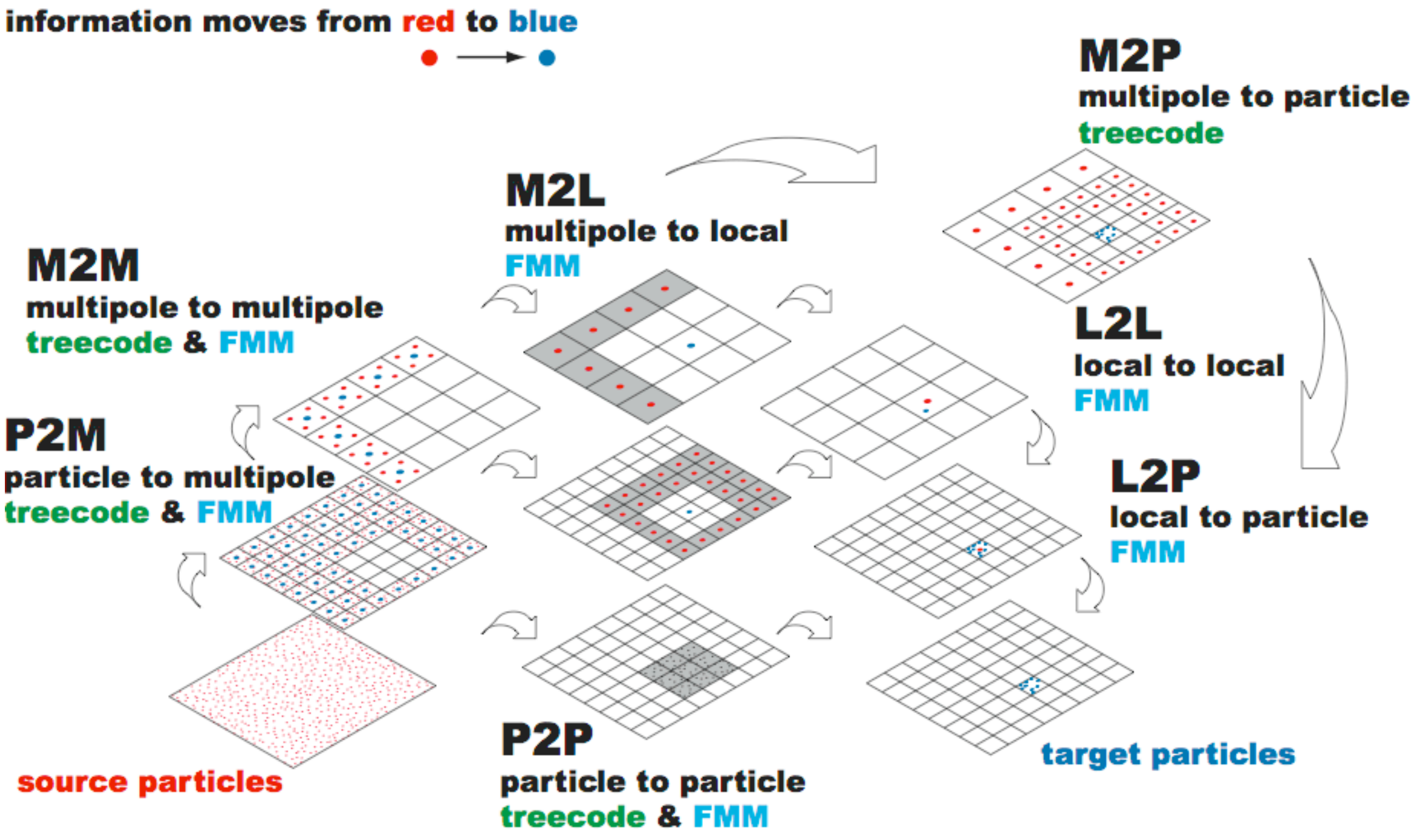
- Computing electrostatic pair interactions between N charges is a common problem
- Computing gravitational forces between N point masses is a nearly equivalent problem
- N is often a 100 000 - 1 000 000 000
- Direct computation: $O(N^2)$
- Particle + mesh methods using FFTs: O(N log N)
- Fast multipole method: O(N)

Fast multipole method



- Compute short-distance interactions directly
- Compute distant interaction as multipole-multipole using multipole expansions centered in the middle of cells
- Use a hierarchical decomposition scheme

FMM: O(N) calculation & communication

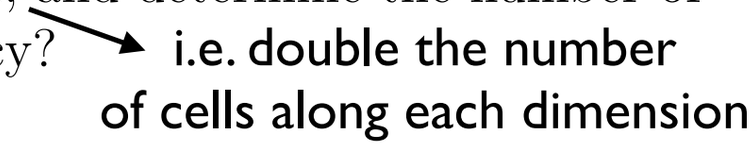


Fast multipole method use

- Example use cases:
  - Galatic dynamics:
    - billions of stars
  - Molecular dynamics
    - ~ a million atoms
  - …
- Different kernels for different problems
- Different requirements: memory versus latency optimization
- Different codes

Projects: Laplace equation

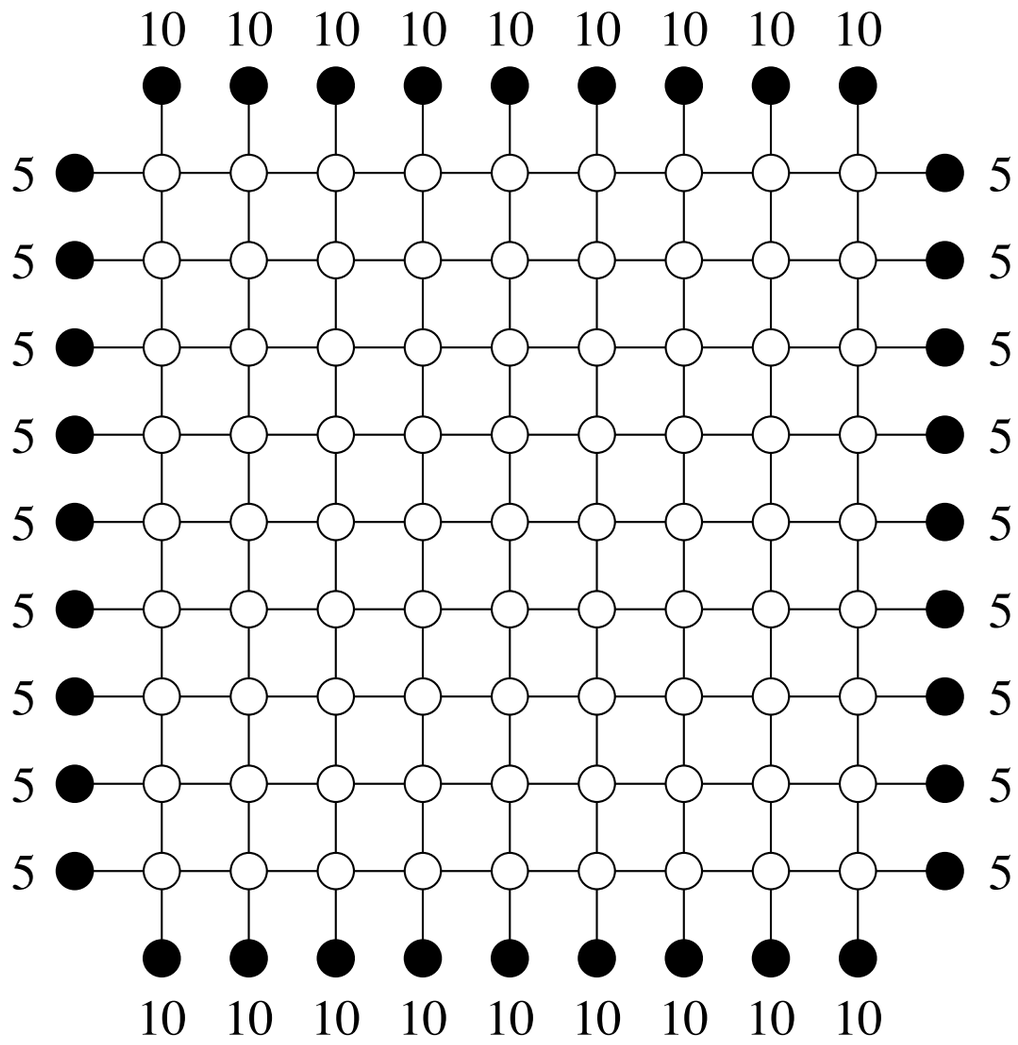
4.1 a) Determine the potential $V(x, y)$ in a square region with linear dimension L=10 (9x9 interior points). The boundary of the square is at a potential $V = 10$. Choose the grid size $\Delta x = \Delta y = 1$. Before you run your program, guess the exact from of $V(x, y)$ and set the initial values of the interior potential 10% lower than the exact answer. How many iterations are necessary to achieve 1% accuracy (max error)? Decrease the grid size $(\Delta x, \Delta y)$ by factor 2, and determine the number of iterations are now necessary to achieve 1% accuracy?



4.1 b) Consider the same geometry as in part a), but set the initial potential at the interior sites equal to zero except for the center site whose potential is set equal to four. Does the potential distribution evolve to the same values as in part a)? What is the effect of a poor initial guess? Are the final results independent of your initial guess?

4.1 c) Modify the boundary conditions so that the value of the potential at the four sides is 5, 10, 5, and 10, respectively (see Figure 10.1). Sketch the equipotential surfaces. What happens if the potential is 10 on three sides and 0 on the fourth? Start with a reasonable guess for the initial values of the potential at the interior

sites and iterate until 1% accuracy is obtained.



Projects: Gauss-Seidel relaxation

4.2 a) Modify the program so that the potential at each site is updated sequentially. That is, after the average potential of the nearest neighbor sites of site i is computed, update the potential at i immediately. In this way the new potential of the next site is computed using the most recently computed values of its nearest neighbor potentials. Are your results better, worse, or about the same as for the simple relaxation method?

4.2 b) Imagine coloring the alternate sites of a grid red and black, so that the grid resembles a checker- board. Modify the program so that all the red sites are updated first, and then all the black sites are updated. This ordering is repeated for each iteration. Do your results converge any more quickly than in part a)?

Projects: Random-walk solution of Laplace's eq.

4.3 a) With the same square region and 5/10/5/10 boundary conditions, compare the results of the random walk method with the results of the relaxation method. Try $n = 100$ and $n = 1000$ walkers, and choose a point near the center of the square.

4.3 b) Repeat part a) for other points within the square. Do you need more or less walkers when the potential near the surface is desired? How quickly do your answers converge as a function of n?

4.4 a) Compute the Green's function $G(x, y, x_b, y_b)$ for the same geometry. Use at least 200 walkers at each interior site to estimate G. Because of the symmetry of the geometry, you can determine some of the values of G from other values without doing an additional calculation. Store your results for G.

4.4 b) Use your results for G found in part a) to determine the potential at each interior site when the 5/10/5/10 boundary potential, except for five boundary sites which are held at $V = 20$. Find the locations of the five boundary sites that maximize the potential at the interior site located at (3,5). Repeat the calculation

to maximize the potential at (5,3). Use trial and error guided by your physical intuition.