

Physics 420: Computational Physics

Fall 2010 Final Exam

Guidelines:

- the exam is to be completed in one sitting of no more than six hours
- students are free to consult their own class notes and to access any other resources available by hyperlink from the class web page
- students may not discuss the contents of the exam with anyone else or use a search engine to troll the internet for answers
- written responses (stored in a file as plain text) and C++ code are to be submitted electronically (bundled in a `.tar.gz` or `.zip` archive) and sent as an attachment to the instructor's email address
- completed exams must be received by Tuesday, December 14, 2010 at 20:00 (hard deadline)

20 points	multiple choice	questions 1–18
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10 points	long answer	questions 19–20
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30 points	programming	questions 21–24
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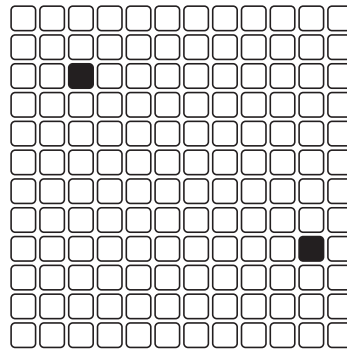
60 points

Multiple Choice Questions (20 points)

Answer by recording one of (a), (b), (c), etc. on the appropriate line of the file `responses.txt`.

1. A cellular automata (CA) system is defined on a square grid of two-state cells (shown below) subject to periodic boundary conditions. Each cell at coordinates (i, j) evolves from one time step t to the next according to a local update rule

$$x_{i,j}^{(t+1)} := F(\{x_{i,j}^{(t)} \text{ and its four nearest neighbours}\}).$$



What is the earliest that the two “on” cells can influence each other?

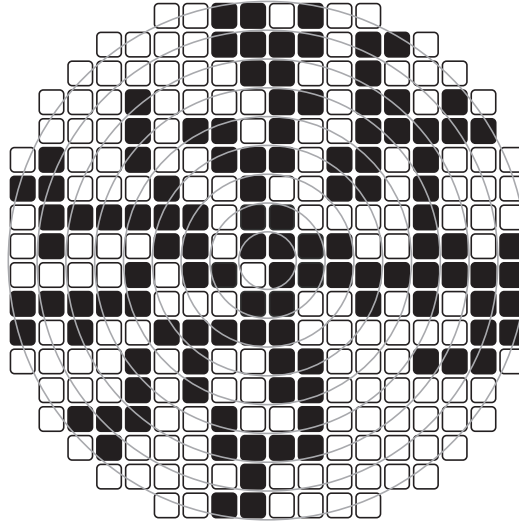
- (a) 5 time steps
 - (b) 7 times steps
 - (c) 10 times steps
 - (d) 14 time steps
 - (e) immediately
2. If, on the other hand, the CA evolves according to

$$x_{i,j}^{(t+1)} := F(\{\text{all sites } x_{k,l}^{(t)}\}),$$

we would say that

- (a) the system has no causal structure
- (b) the relationship between events cannot be categorized as either space-like or time-like
- (c) all cells influence all others with no time lag
- (d) all of the above

3. A process called *diffusion-limited aggregation* produces the following small cluster.



The number of cells that are “on” in each concentric ring of radius R is tabulated below.

radius (R)	count (C)	area (πR^2)
1	3	3.142
2	10	12.57
3	19	28.27
4	30	50.27
5	44	78.54
6	59	113.1
7	76	153.9
8	96	201.1
9	117	254.5

Which of the following is true?

- (a) The cluster is contiguous with respect to connectivity defined by neighbours in the four cardinal directions.
- (b) The cluster has fractal dimension $d_f = 1/3$.
- (c) A plot of the data, presented as $\log C$ versus $\log R$, can be fit by a straight line of slope $5/3$.
- (d) The cluster has fractal dimension $d_f = 7/3$.
- (e) The cluster has all the symmetries of the underlying square lattice.

4. In conventional mathematical notation, the matrix

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ \vdots & & & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{pmatrix}$$

has elements $A_{i,j}$ indexed by row $i = 1 \dots m$ and column $j = 1 \dots n$. Consider the special case where A is an $N \times N$ square and is anti-symmetric, so that its elements obey $A_{i,j} = -A_{j,i}$ for all $1 \leq i, j \leq N$.

For efficiency, we might want to store only those $N(N - 1)/2$ elements that are not redundant. Let's pack them into a C array by storing the non-diagonal, upper triangular elements of A in row-major order—i.e.,

$$\boxed{A_{1,2} \mid A_{1,3} \mid \dots \mid A_{1,N} \mid A_{2,3} \mid A_{2,4} \mid \dots \mid A_{2,N} \mid \dots \mid A_{N-2,N-1} \mid A_{N-2,N} \mid A_{N-1,N}}$$

—and then devise an indexing rule that respects the 1-based indexing. What is the correct replacement for ... in the following program?

```
#include <cstddef>
using std::size_t;

const size_t N = 9;
double Adata[N*(N-1)/2];

double A(size_t i, size_t j)
{
    if (i == j) return 0.0;
    else if (i < j) return ... ;
    else return -A(j,i)
}

int main()
{
    double sum = 0.0;
    for (size_t i = 1; i <= N; ++i)
        for (size_t k = 1; k <= N; ++k)
            sum += A(i,k)*A(k,i);
    return 0;
}
```

- (a) `Adata[(i-1)*N+j-1]`
- (b) `Adata[j-i-1+(2*N-i)*(i-1)/2]`
- (c) `Adata[j*(j-1)+(i-1)*N]`
- (d) `Adata[(i+1)*(j-1)/2]`

5. What does the code in question 4 actually compute? (Specifically, what value is held in `sum` when `main` terminates.)

- (a) $(\text{tr } A)^2$
- (b) $\text{tr } A^2$
- (c) $(\det A)^2$
- (d) $\det A^2$

6. A field ϕ in two-dimensional space is restricted to a square grid of points, uniformly spaced by $\Delta x = \Delta y$: i.e., $\phi(i \cdot \Delta x, j \cdot \Delta x) = \phi_{i,j}$. Which of the following is not an appropriate finite-difference approximation to the Laplacian $\nabla^2 \phi$?

- (a) $\frac{1}{(\Delta x)^2} [\phi_{i+1,j} + \phi_{i,j+1} + \phi_{i-1,j} + \phi_{i,j-1} - 4\phi_{i,j}]$
- (b) $\frac{1}{2(\Delta x)^2} [\phi_{i+1,j+1} + \phi_{i-1,j+1} + \phi_{i-1,j-1} + \phi_{i+1,j-1} - 4\phi_{i,j}]$
- (c) $\frac{1}{(2\Delta x)^2} [\phi_{i+2,j+1} + \phi_{i-2,j+1} + \frac{2}{3}\phi_{i,j-3} - \frac{8}{3}\phi_{i,j}]$
- (d) $\frac{1}{(3\Delta x)^2} [\phi_{i+2,j+1} + \phi_{i-2,j+1} + \phi_{i+1,j-2} + \phi_{i-1,j-2} - 4\phi_{i,j}]$

7. A quantum particle living in one dimension is characterized by its wavefunction $\psi(x)$. Suppose that the continuous spatial coordinate $x \in \mathbb{R}$ is approximated by a uniform mesh, so that the wave function $\psi_i = \psi(x_i)$ is evaluated only at discrete points $x_i = i \cdot a$ (for integer i). A symmetric finite difference expression for the kinetic energy is as follows:

$$\hat{E}_{\text{kin}}\psi(x) = \frac{1}{2m}\hat{p}^2\psi(x_i) = -\frac{\hbar^2}{2m}\left.\frac{\partial^2\psi(x)}{\partial x^2}\right|_{x=x_i} \approx -\frac{\hbar^2}{2ma^2}(\psi_{i-1} + \psi_{i+1} - 2\psi_i).$$

If the particle interacts with nothing else and is subject to no confining potential, then it is free and has a plane wave form with wavevector k . The single-particle energy is

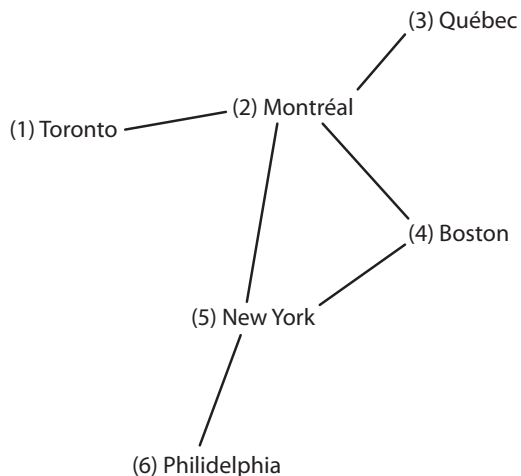
- (a) $\hbar^2 k / 2ma$
- (b) $\hbar^2 k^2 / 2m$
- (c) $(\hbar^2 / ma^2)(1 - \cos ka)$
- (d) $(\hbar^2 k / 2ma) \sin ka$

8. For question 7, in what parameter regime is the continuum result recovered?

- (a) $m \rightarrow 0$
- (b) $\hbar \rightarrow 0$
- (c) $a \ll 1/k$
- (d) $a \gg 1/k$

The next four questions relate to the following Monte Carlo problem.

A confused and aimless passenger travels on the train network shown below.



Each day she moves from one city to the next according to the transition matrix

$$T = \begin{pmatrix} 0 & a & 0 & 0 & 0 & 0 \\ a' & 0 & b & c & d & 0 \\ 0 & b' & 0 & 0 & 0 & 0 \\ 0 & c' & 0 & 0 & e & 0 \\ 0 & d' & 0 & e' & 0 & f \\ 0 & 0 & 0 & 0 & f' & 0 \end{pmatrix}.$$

The elements $T_{ij} = \text{Prob}(j \rightarrow i)$ denote the probability of going from city j to city i .

9. (2 points) Which of the following statements about the traveller are true and false?
 - (t / f) She never stays in one place more than a day.
 - (t / f) She always disembarks when her train enters a new city.
 - (t / f) If she starts in Toronto she can never reach Philidelphia.
 - (t / f) If she starts in Québec she can never return to it unless $b' \neq 0$.
10. Which of the following is *not* a necessary condition for T to serve as a transition matrix?
 - (a) $f = 1$
 - (b) $d = d'$
 - (c) $c + e' = 1$
 - (d) $e \geq 0$

11. Suppose we use T to generate a Markov chain representing the passenger's daily travel. We find that in the long-time limit the passenger spends one third of her time in Montréal, Boston, and New York and a vanishing fraction of time in the remaining cities. In other words, the steady-state distribution looks like this:

$$\lim_{N \rightarrow \infty} \pi^{(N)} = \lim_{N \rightarrow \infty} T^N \pi^{(0)} = \pi^* = \begin{pmatrix} 0 \\ 1/3 \\ 0 \\ 1/3 \\ 1/3 \\ 0 \end{pmatrix}$$

Which values are *not* consistent with this?

- (a) $a = b' = c = d' = e = f' = 0$ and $c' = d = e' = 1$
 (b) $a = b' = c' = d = e' = f' = 0$ and $c = d' = e = 1$
 (c) $a = b' = f' = 0$ and $c = c' = d = d' = e = e' = 1/2$
12. What is the correct statement of *detailed balance*?
- (a) $T_{ij}\pi_j^* = T_{ji}\pi_i^*$
 (b) $T_{ij} = T_{ji}$
 (c) $\sum_j T_{ij}\pi_j^* = \pi_i^*$
13. (2 points) Here is a program that performs various double-precision floating-point operations.

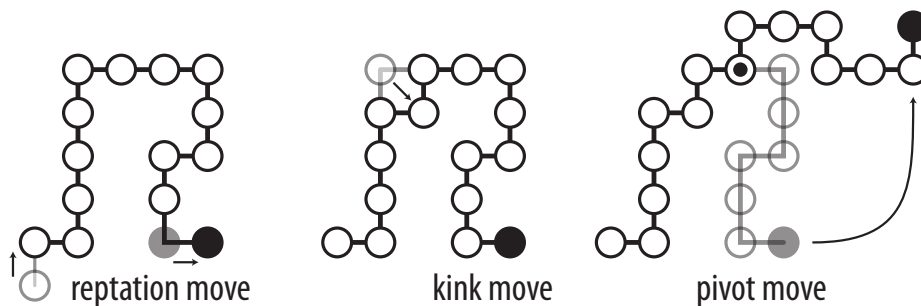
```
int main()
{
    double a = 2.0;
    while (1.0/a > 0.0) a *= a;
    const double b = -5.0/a;
    const double c = a/b;
    const double d = a+c;
    const double e = a*b;
    return 0;
}
```

Which of the following are true or false statements about the state of memory when the program terminates?

- (t / f) **a** has value `inf`
 (t / f) **b** has value `0.0`
 (t / f) **c** has value `-inf`
 (t / f) **d** has value `0.0`
 (t / f) **e** has value `nan`

For the next two questions, answer by writing the corresponding letter in the spaces provided. Each of (a), (b), (c) [and (d) for question 15] should appear at most once.

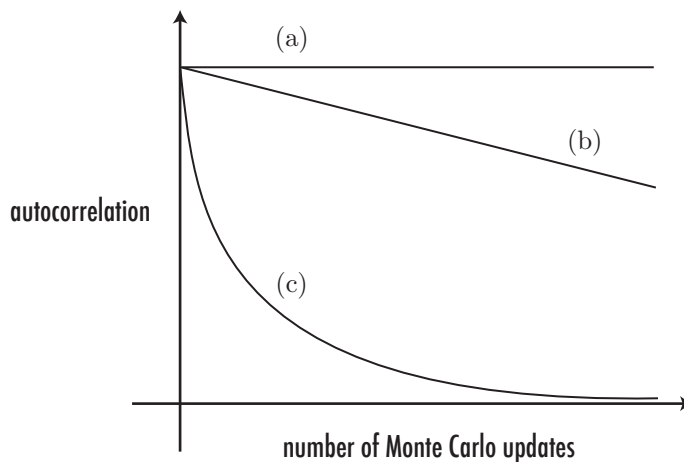
14. A long self-avoiding walk (SAW) of fixed length is sampled via Monte Carlo using the update rules show below.



A large number M of updates are performed, and the end-to-end distance of the SAW is measured after each one, yielding a set of observations $\{r(0), r(1), r(2), \dots, r(M)\}$. Each $r(m) > 0$ is the distance after m updates have been performed. For $M \gg n$, the r -autocorrelation is approximately

$$C_r(n) \approx \frac{1}{M-n+1} \sum_{m=0}^{M-n} r(n+m)r(m) - \left(\frac{1}{M+1} \sum_{m=0}^M r(m) \right)^2.$$

Which update schemes correspond to the autocorrelation behaviour show here?

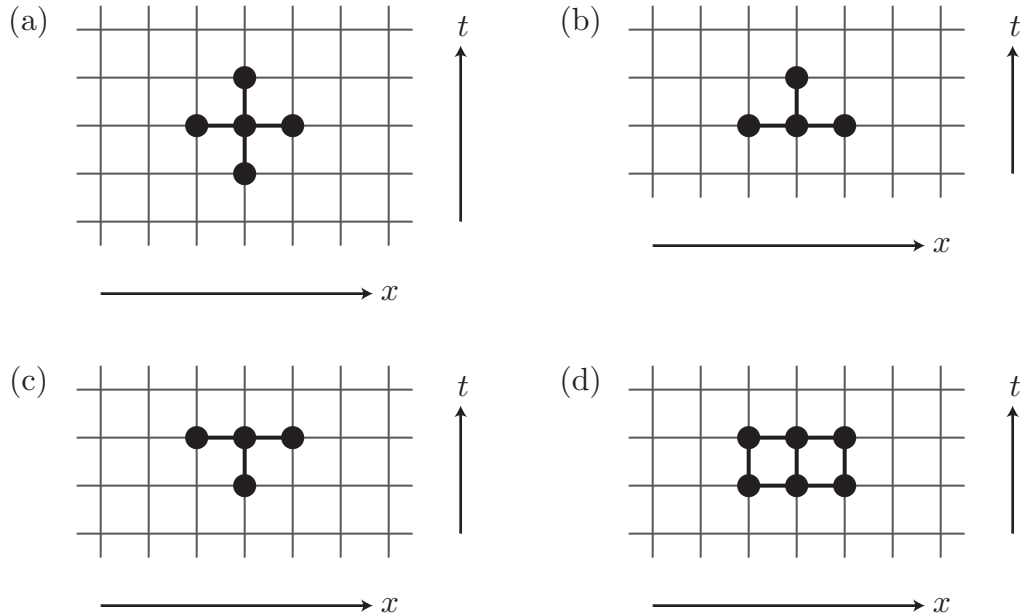


- (a) a combination of reptation and kink moves
- (b) kink moves only
- (c) pivot moves only

15. The field $u(x, t)$ is evaluated at a mesh of points $u_i^{(n)} = u(i \cdot \Delta x, n \cdot \Delta t)$ in order to build a finite difference approximation to the partial differential equation

$$\frac{\partial u(x, t)}{\partial t} = D \frac{\partial^2 u(x, t)}{\partial x^2}.$$

Which of the following four *stencils*



correspond to these three systems of equations:

- (___) $u_i^{(n+1)} = (1 - 2s)u_i^{(n)} + s(u_{i+1}^{(n)} + u_{i-1}^{(n)})$
- (___) $(1 + 2s)u_i^{(n+1)} - s(u_{i+1}^{(n+1)} + u_{i-1}^{(n+1)}) = u_i^{(n)}$
- (___) $(1 + s)u_i^{(n+1)} - \frac{s}{2}(u_{i+1}^{(n+1)} + u_{i-1}^{(n+1)}) = (1 - s)u_i^{(n)} + \frac{s}{2}(u_{i+1}^{(n)} + u_{i-1}^{(n)})$

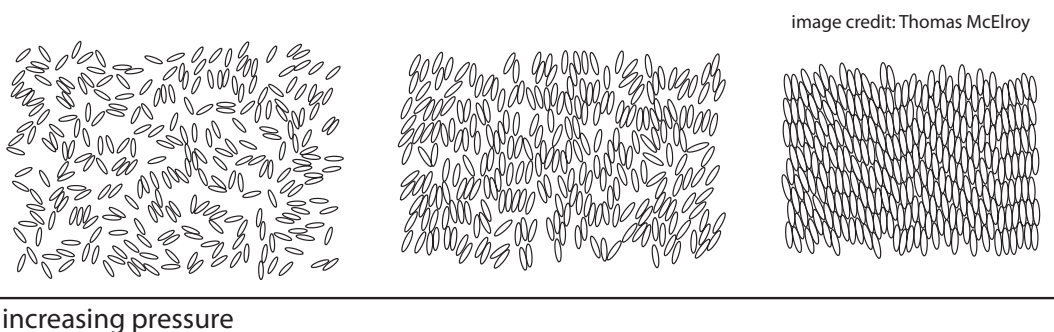
16. Which of the four stencils in question 15 depicts an *explicit* integration scheme?

- (a)
 (b)
 (c)
 (d)
 (e) none of them

17. Consider a finite collection of N hard ellipses (contained in a square box with periodic boundary conditions) that are completely independent except for excluded volume interactions. The ellipses are all identical and are in the limit $a \gg b$, where a and b are the lengths of the major and minor axes. At low pressure, when the density of ellipses is low, the ellipses behave as an ideal gas (but with internal rotational degrees of freedom, just like diatomic molecules). The ellipses are largely uncorrelated beyond a few lengths a .

At extremely high pressure, the ellipses are tightly packed and tend to order like a crystalline solid. In other words, there is strong orientational and positional correlation between ellipses.

At moderate pressure, there is an intermediate phase—called a *nematic* or *liquid crystal*—that preserves the translational symmetry of the gas but exhibits long-range orientational order (which is to say that the rods tend to align).



Let \mathbf{r}_i be the position of each ellipse in the x - y plane and $\mathbf{n}_i = (\cos \theta_i, \sin \theta_i)$ a unit vector directed along the line connecting each ellipse's two foci. Suppose we measure these two quantities:

$$g_1 = \sum_{i < j} \left(\langle \mathbf{n}_i \cdot \mathbf{n}_j \rangle - \langle \mathbf{n}_i \rangle \cdot \langle \mathbf{n}_j \rangle \right)$$

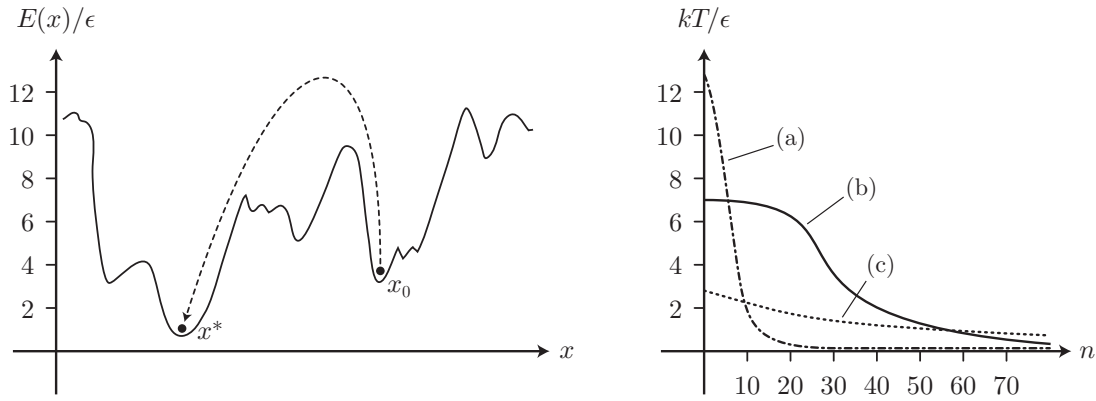
$$g_2 = \sum_{i < j} \langle \cos [2(\theta_i - \theta_j)] \rangle$$

Which of the following signals that the system has nematic order?

- (a) $\lim_{N \rightarrow \infty} g_1 = 1$
- (b) $g_1 = N^2$
- (c) $g_2 = N(N - 1)/2$
- (d) $\lim_{N \rightarrow \infty} g_2/N^2 \neq 0$

18. A thermal walker—at position x_n and temperature T_n after n steps—moves through the energy landscape $E(x)$. A large barrier separates its initial position x_0 from the global minimum at x^* . The walker attempts steps of the form $x_{n+1} := x_n + r\Delta x$, where r is a number drawn randomly from the uniform distribution on $[-1, 1]$ and $\Delta x \approx |x^* - x_0|/20$. (If the attempt is rejected, then $x_{n+1} := x_n$)

The plot on the right shows three possible cooling schedules. Which of the three is most likely to allow the walker to make the journey from x_0 to x^* ?



- (a)
- (b)
- (c)
- (d) none of them can ever make it over the energy barrier

Long Answer Questions (10 points)

19. (4 points) Read over the following C++ class definition.

```
#include <iostream>
using std::ostream;
using std::endl;

template <typename T>
class accml8r
{
private:
    T x2, x4, x6;
    unsigned long int c;
public:
    accml8r() : x2(0), x4(0), x6(0), c(0) {}
    accml8r(T x2_, T x4_, T x6_, unsigned long int c_) :
        x2(x2_), x4(x4_), x6(x6_), c(c_) {}
    void capture(T v)
    {
        const T v2 = v*v;
        const T v4 = v2*v2;
        x2 += v2; x4 += v4; x6 += v2*v4; ++c;
    }
    void reset(void) { x2 = x4 = x6 = 0; c = 0; }
    friend ostream& operator<<(ostream &os, const accml8r<T> &A)
    {
        if (A.c == 0)
            os << "0\t0\t0" << endl;
        else
            os << A.x2/A.c << "\t" << A.x4/A.c << "\t" << A.x6/A.c << endl;
    }
    friend accml8r<T> operator+(const accml8r<T> &A, const accml8r<T> &B)
    {
        return accml8r(A.x2+B.x2,A.x4+B.x4,A.x6+B.x6,A.c+B.c);
    }
};
```

- (a) Explain what the `accml8r` class does.
- (b) What role might an object of type `accml8r<int>` play in a Monte Carlo simulation of the Ising ferromagnet.
- (c) There's at least one coding error. Please identify it. (Hint: one of `accml8r<int>` and `accml8r<double>` behaves incorrectly.)
- (d) Suppose you've written a Wolff algorithm code that samples the magnetization $M = \sum_i s_i$ (with $s_i = \pm 1$) in a square $L \times L$ system; you're running the simulation at low temperature (near ferromagnetic saturation) and trying to measure the Binder ratio $B = \langle M^4 \rangle / \langle M^2 \rangle^2$. If you're accumulating values in an `int`, working on a machine in which `sizeof(int) = 2`, and you want at least 50 measurements per bin, what's the maximum value of L that can be simulated?

20. (6 points) Consider a system of N charged particles governed by the classical Hamiltonian

$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} \frac{e^2(-1)^{i+j}}{4\pi\epsilon_0\sqrt{r_{ij}^2 + a^2}} + \sum_{i=1}^N e(-1)^i \mathcal{E}_0 x_i$$

and confined to an $L \times L \times L$ box (with reflecting walls rather than periodic boundary conditions). The particles have charge $q_i = e(-1)^i$ and interact via an electrostatic potential cut off by a small length scale a ; an electric field \mathcal{E}_0 is applied between the two planes coinciding with the walls at $x = 0$ and $x = L$.

(a) How many particles have charge $+e$?

(b) Hamilton's equations tell us that $\dot{\mathbf{p}}_i = -\partial H/\partial \mathbf{r}_i$. Explain why two oppositely-charged particles separated a distance $r_{ij} \ll a$ feel a linear restoring force with a Hooke's law constant $K = \pm e^2/4\pi\epsilon_0 a^3$.

(c) Suppose that the container walls are held fixed at temperature T and serve as a heat bath for the system of particles. How do the particles behave when $k_B T$ is the largest energy scale in the problem?

(d) How do the particles behave when $e\mathcal{E}_0 L$ is the largest energy scale in the problem?

(e) Describe the particle behaviour in the limit $T \ll e\mathcal{E}_0L \ll e^2/4\pi\epsilon_0a$.

(f) In a computer simulation, what is the effect of taking $a \rightarrow 0$ on the total computational effort? Comment on energy conservation and the choice of time step.

Programming (30 points)

I recommend that you complete this section of the exam in the computer lab. You are free to organize your program in any way you choose so long as all the code resides in the program file `potential.cpp` and can be compiled with the provided `makefile`.

To start, download the `Exam.tar.gz` archive from the exam start page:

http://www.ualberta.ca/~kbeach/phys420_exam.html

Unpack the archive and append your own last name to the `Exam` directory.

```
$ tar xzf Exam.tar.gz
$ mv Exam Exam_StudentLastName
$ cd Exam_StudentLastName
```

At the end of the exam, you should archive your work directory. Please remember to first remove the executables and `outputxxxx.dat` files with `make clean`. Be absolutely sure that `responses.txt` is included.

```
$ make clean
$ cd ..
$ tar czf Exam_StudentLastName.tar.gz Exam_StudentLastName
```

Email it to the instructor at `kbeach@ualberta.ca`.

Imagine an experimental setup in which two localized electronic orbitals, each carrying net negative charge $-e$, lie on the surface of a material some distance R apart. If the spatial extent of the occupied orbitals were negligible, we would describe them as point charges

$$\rho = -e\delta(\mathbf{r} - R\hat{y}/2) - e\delta(\mathbf{r} + R\hat{y}/2).$$

Here, though, we're going to assume that the charge in each of the orbitals is smeared out like a gaussian over some characteristic length σ (as per the function `init`).

If the material had no substantial dielectric response, the electrostatic potential would be described by Laplace's equation,

$$\nabla^2\phi = \frac{\rho}{\epsilon_0}.$$

Working in units where $\epsilon_0 = 1$, the discretized version of this equation is

$$(A) \quad \phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - 4\phi_{i,j} = (\Delta x)^2\rho_{i,j}.$$

This assumes a square grid with uniform spacing $\Delta x = \Delta y$.

More generally, the potential is described by

$$\nabla \cdot (\epsilon \nabla \phi) = \rho,$$

which does not reduce to Laplace's equation if the dielectric constant is position-dependent. That's the case here, since the dielectric constant changes abruptly across the edge of the material:

$$(B) \quad \epsilon(x, y) = \epsilon_0 + (\epsilon_{\text{bulk}} - \epsilon_0)[1 - \tanh(x/\sigma)]/2.$$

We'll use the values $\epsilon_0 = 1$ and $\epsilon_{\text{bulk}} = 14$.

21. (6 points) The program `potential.cpp` is very rudimentary. It initializes the electrostatic potential with random values and then performs 50 relaxation steps derived from Equation (A). (Note the ϕ is held at zero everywhere on the edge of the simulation region.) The `movie.gp` script shows the evolution over those steps, and `final.gp` shows the final state only.

```
$ make
g++ -o potential potential.cpp -O2 -ansi -pedantic
$ ./potential
usage: potential R sigma
$ ./potential 6.0 1.0
$ gnuplot movie.gp
$ gnuplot final.gp
```

Modify the program so that relaxation continues until each cell is converged to at least one part in 10^4 . (You may want to reduce the frequency at which the `outputxxxx.dat` files are created: a snapshot of every 10th update, say.)

22. (10 points) Extend `potential.cpp` so that it correctly handles the position-dependent form of $\epsilon(x, y)$ given in Equation (B). You'll have to think about how to discretize $\nabla \cdot (\epsilon \nabla \phi)$.
23. (7 points) Make a vector plot of the electric field $\mathbf{E} = \nabla \phi$ and the displacement field $\mathbf{D} = \epsilon \nabla \phi$ for $R = 6$ and $\sigma = 1$.
24. (7 points) Compute the energy contained in the field

$$\int dx dy \frac{1}{\epsilon} |\epsilon \nabla \phi|^2$$

as a function of the separation R . Plot the R dependence for σ values $1/4$, $1/2$, and 1 .