Lattice gas simulations

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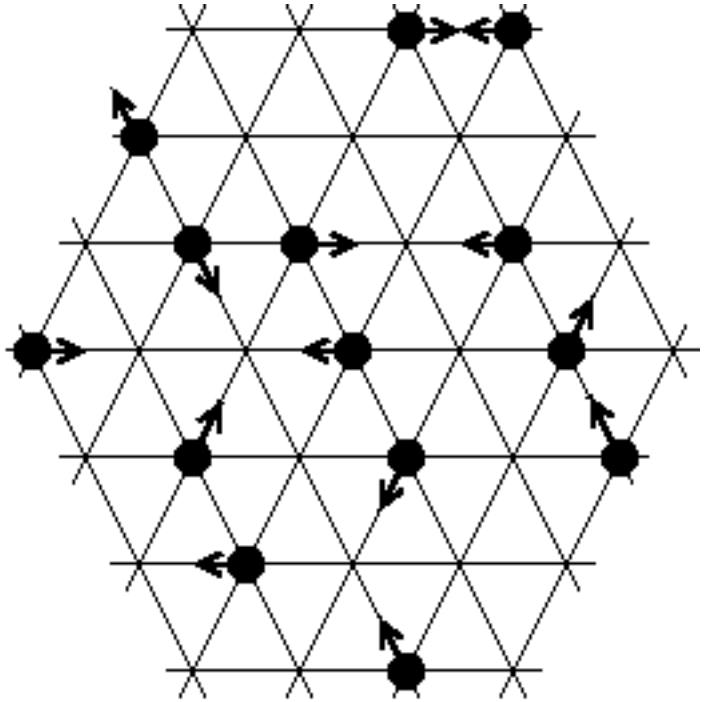
18.354 Project

Overview

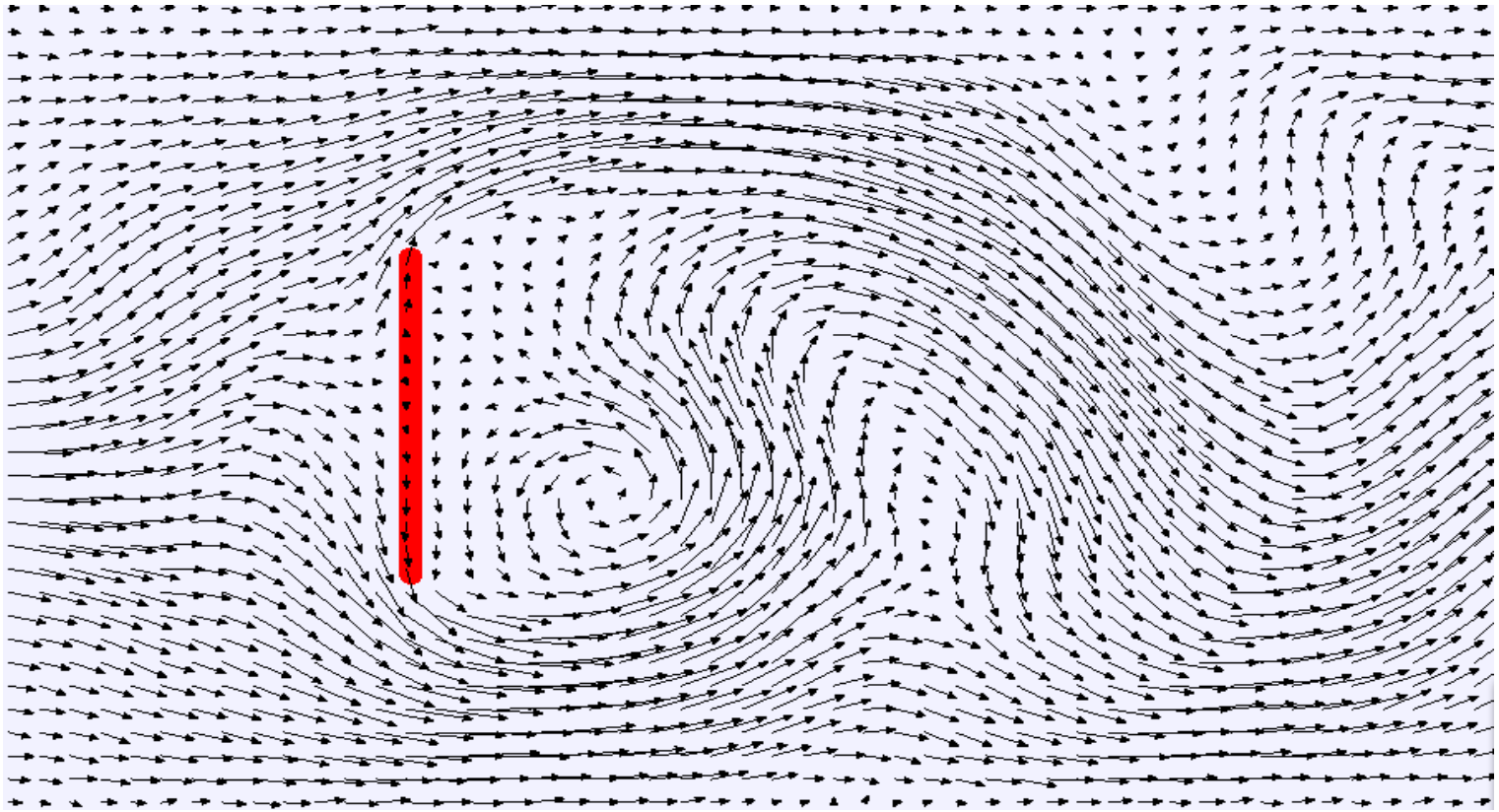
1. Introducing the lattice gas;
2. Analytic description of the lattice gas;
3. Program objectives;
4. How to implement it (efficiently);
5. Demonstrations;

What is the lattice gas?



- A completely unphysical description of the motion of particles.
- The lattice gas particle is an entity that hops from point to point on the lattice with each (discrete) time step.

Why do we use it?



- Despite its artificial nature, very physical results arise when observed at large enough scales.

Why do we use it? (2)

- Because trying to simulate a collection of particles in continuous space is expensive.
- Intuitively, the problem scales as $O(n^2)$ just for the collisions.
  - For each of the n particles,
  - we have to test whether it has collided with (n-1) other particles.
  - Actually, the situation is more complicated: How do we detect for three-body collisions, for instance?
- We'll see later that the lattice gas has nice scaling properties in terms of the required computational effort.

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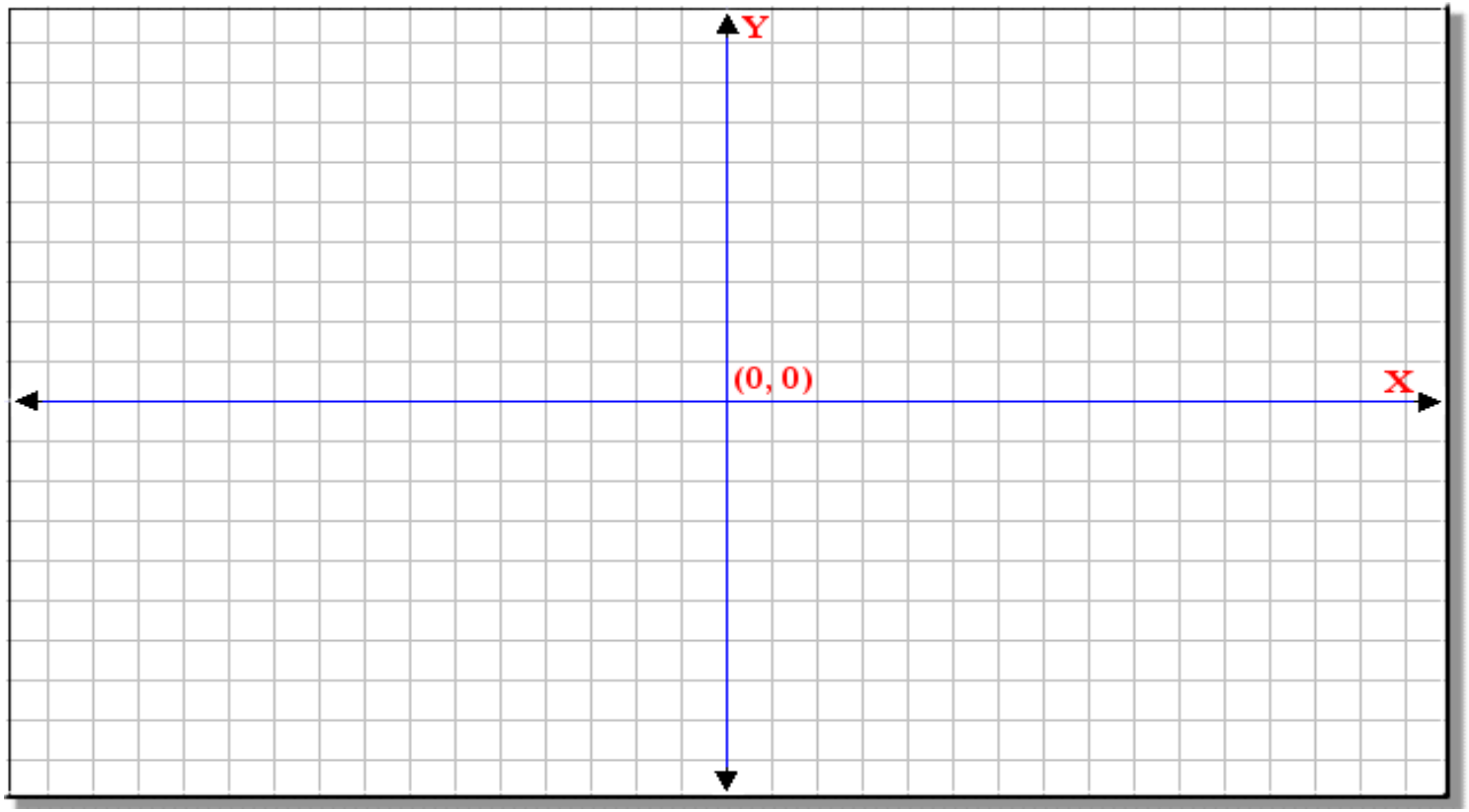
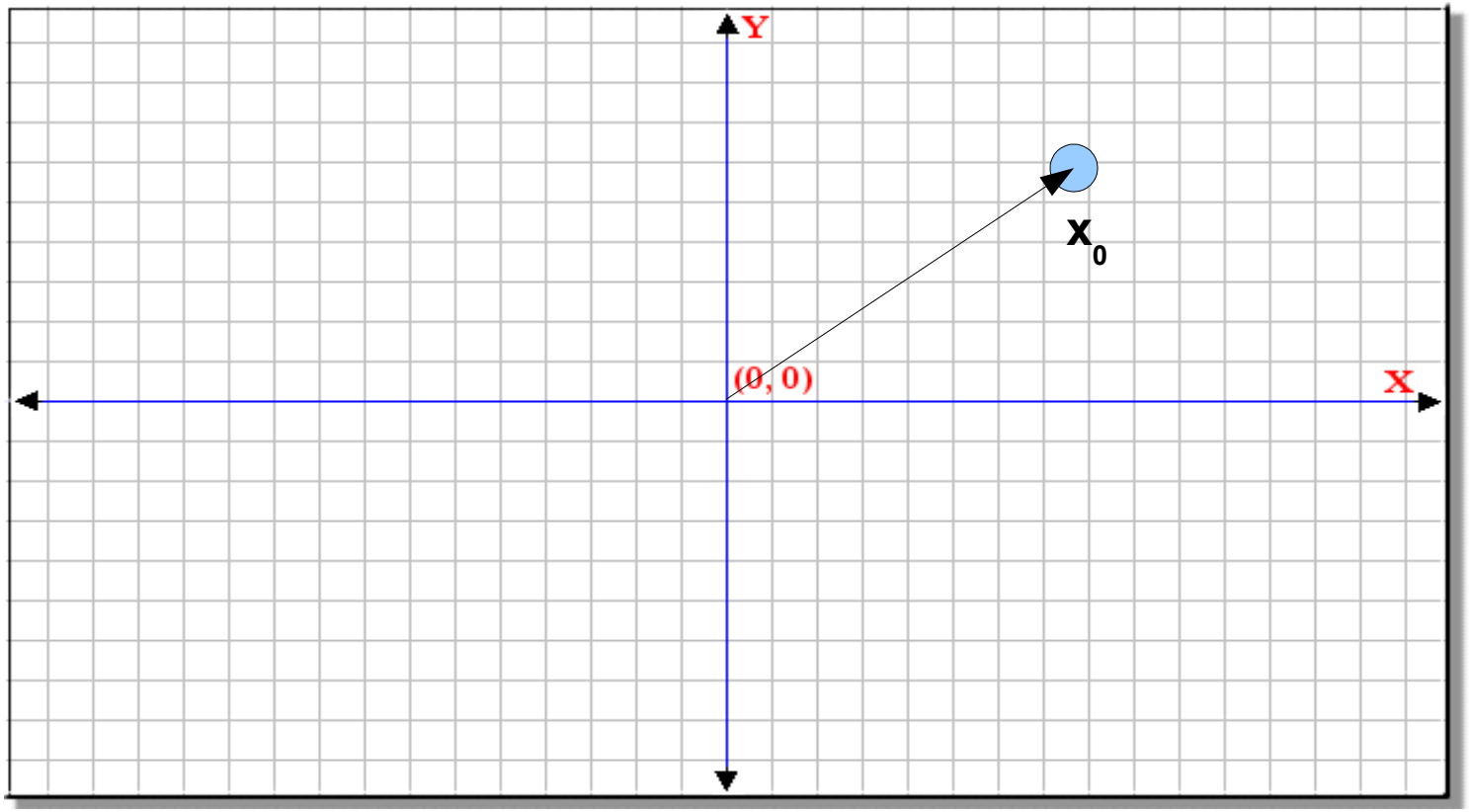
How do we describe the lattice network?



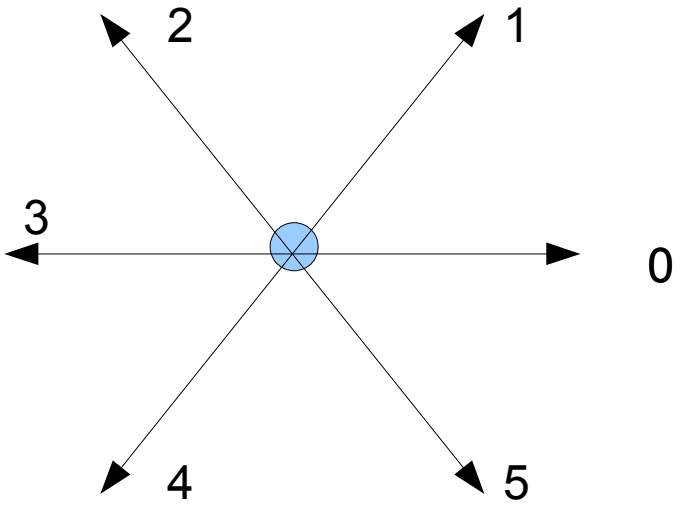
First, start with an empty coordinate plane

Place a node at position $\mathbf{x}_0$



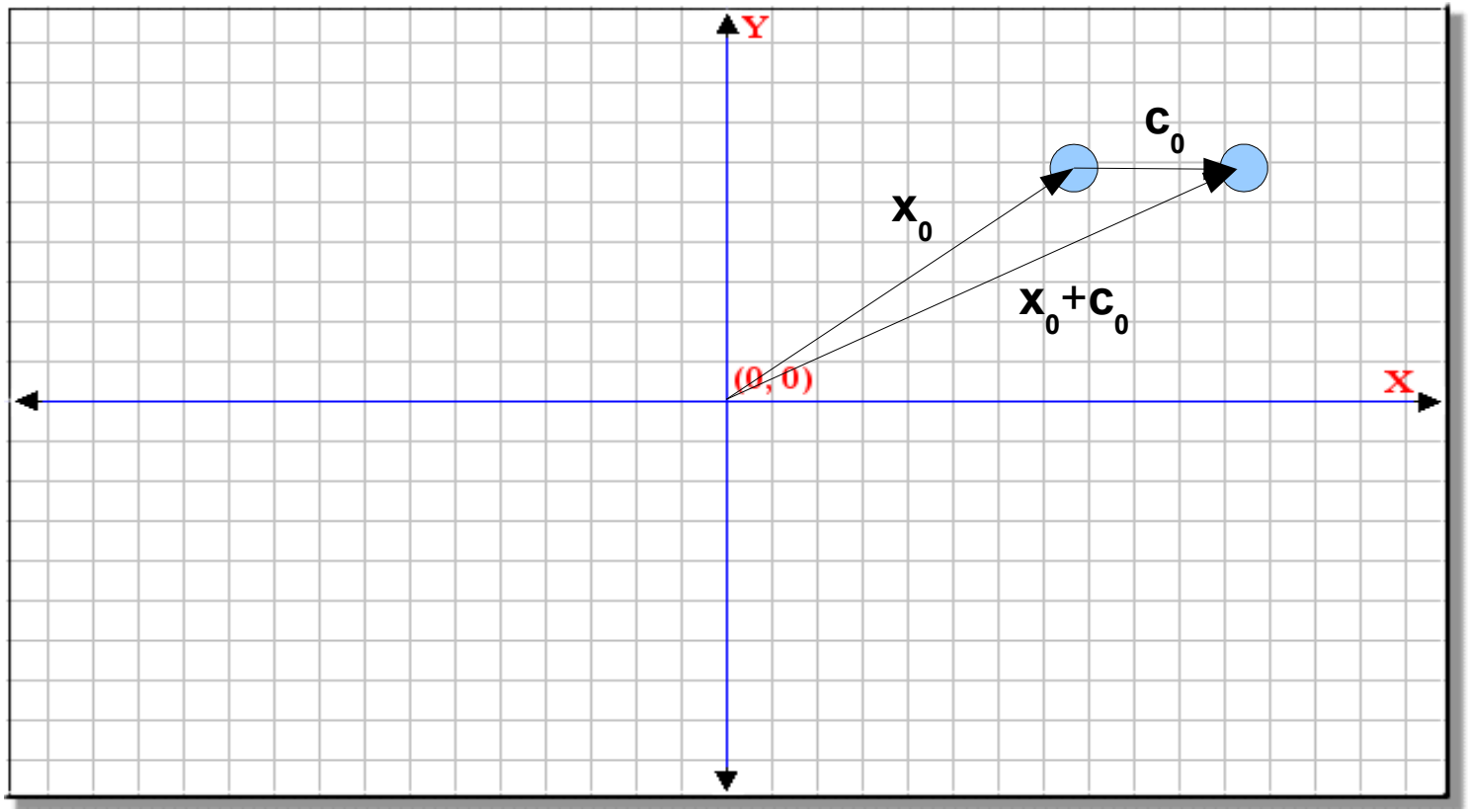
- We now use $\mathbf{x}_0$ to label the node *at* $\boldsymbol{x}_0$.
  - *We can refer to the node at* $\boldsymbol{x}_0$ *by the vector.*

One point is no lattice; so let's add some neighbors



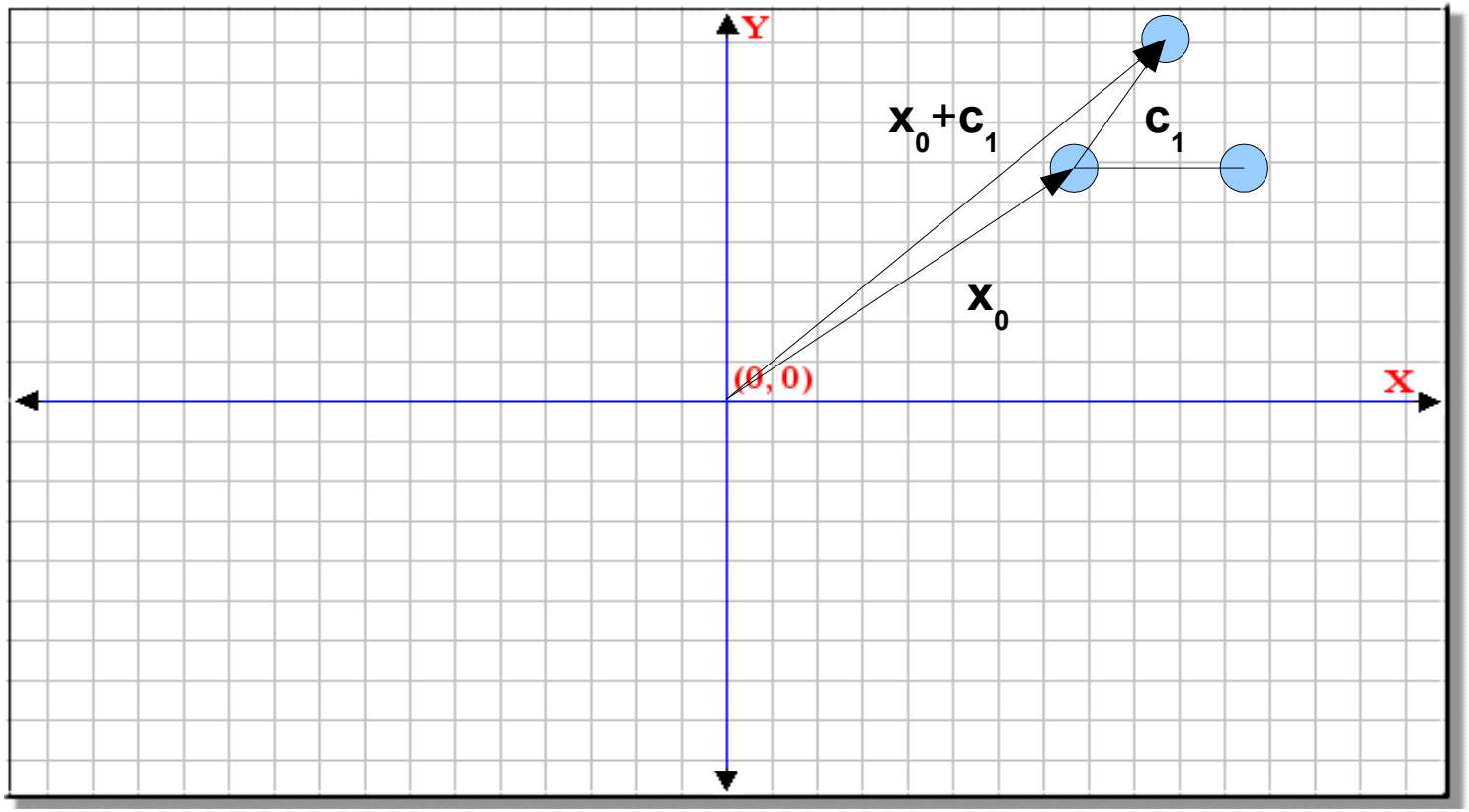
- Let $\mathbf{c}_i$ denote the vector that connects a node to its neighbor in the i-th direction,
  - where i = 0, 1, 2, 3, 4, 5; (see above)

Creating neighbors



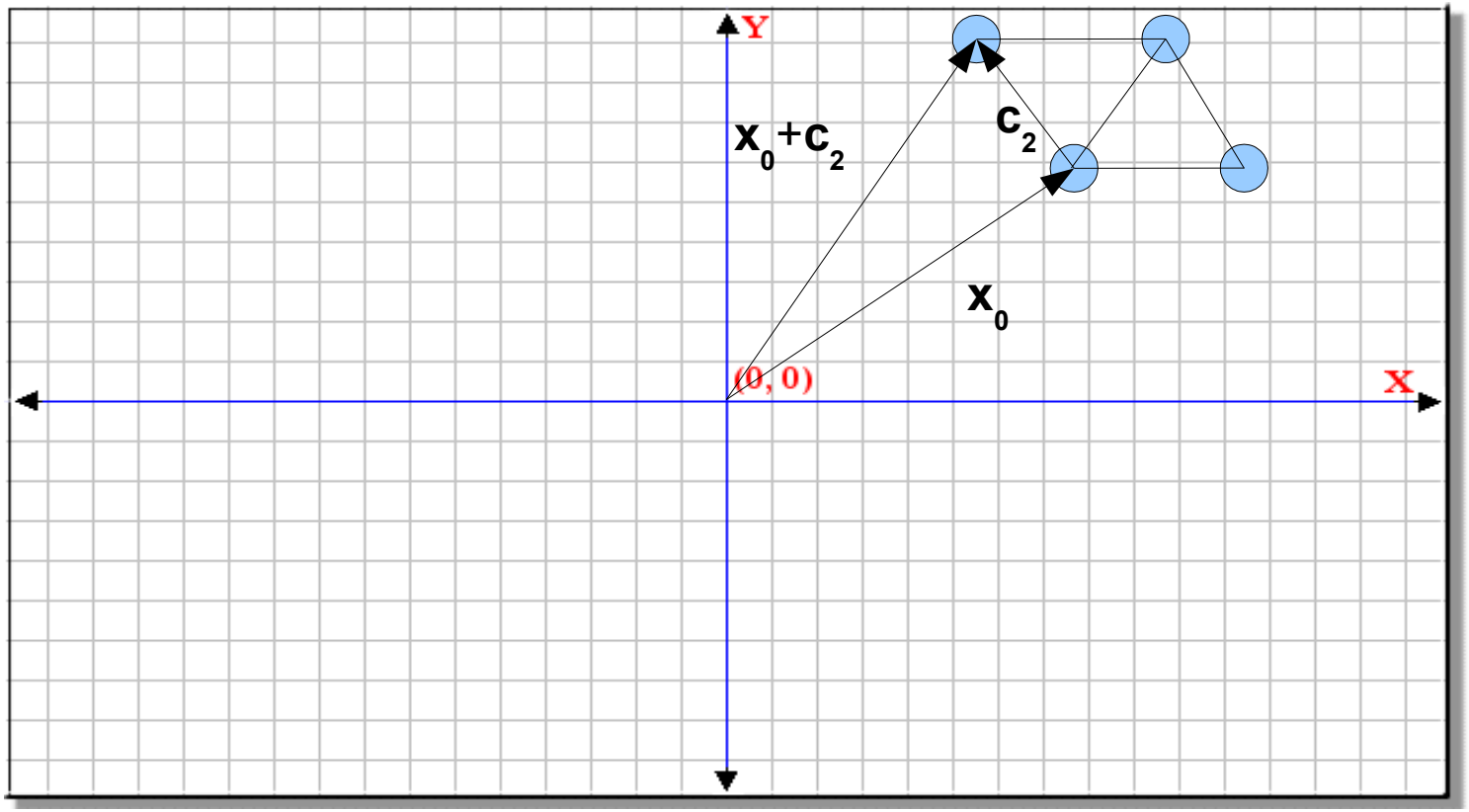
- So we can add a new node at $\mathbf{x_0 + c_0}$
- The new node too can be identified by its position in the coordinate system: $\mathbf{x_0 + c_0}$

And so on ($\mathbf{x_0 + c_1}$)...

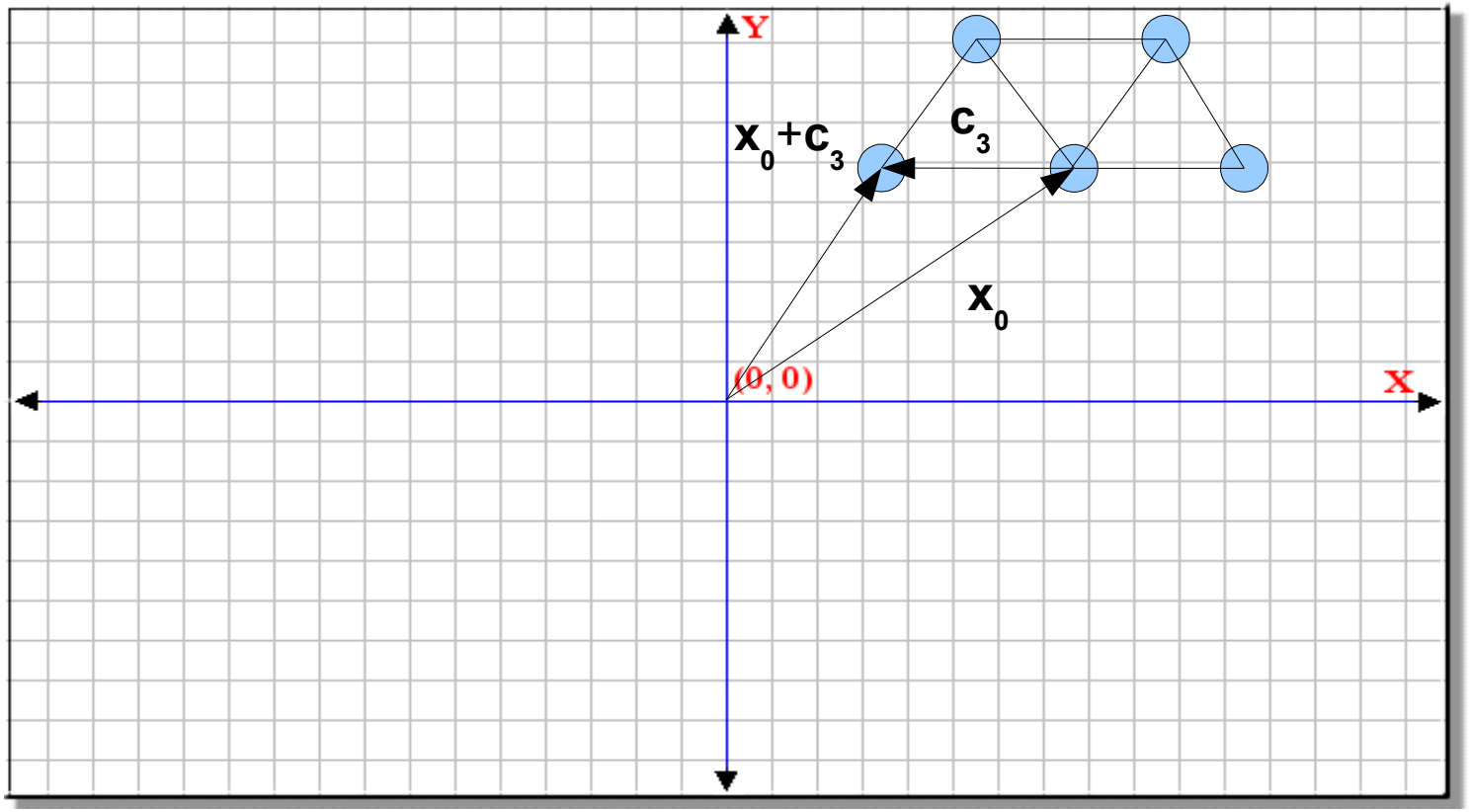


- The solid line indicates a “lattice connection” between the node at $\mathbf{x_0}$ and $\mathbf{x_0 + c_0}$

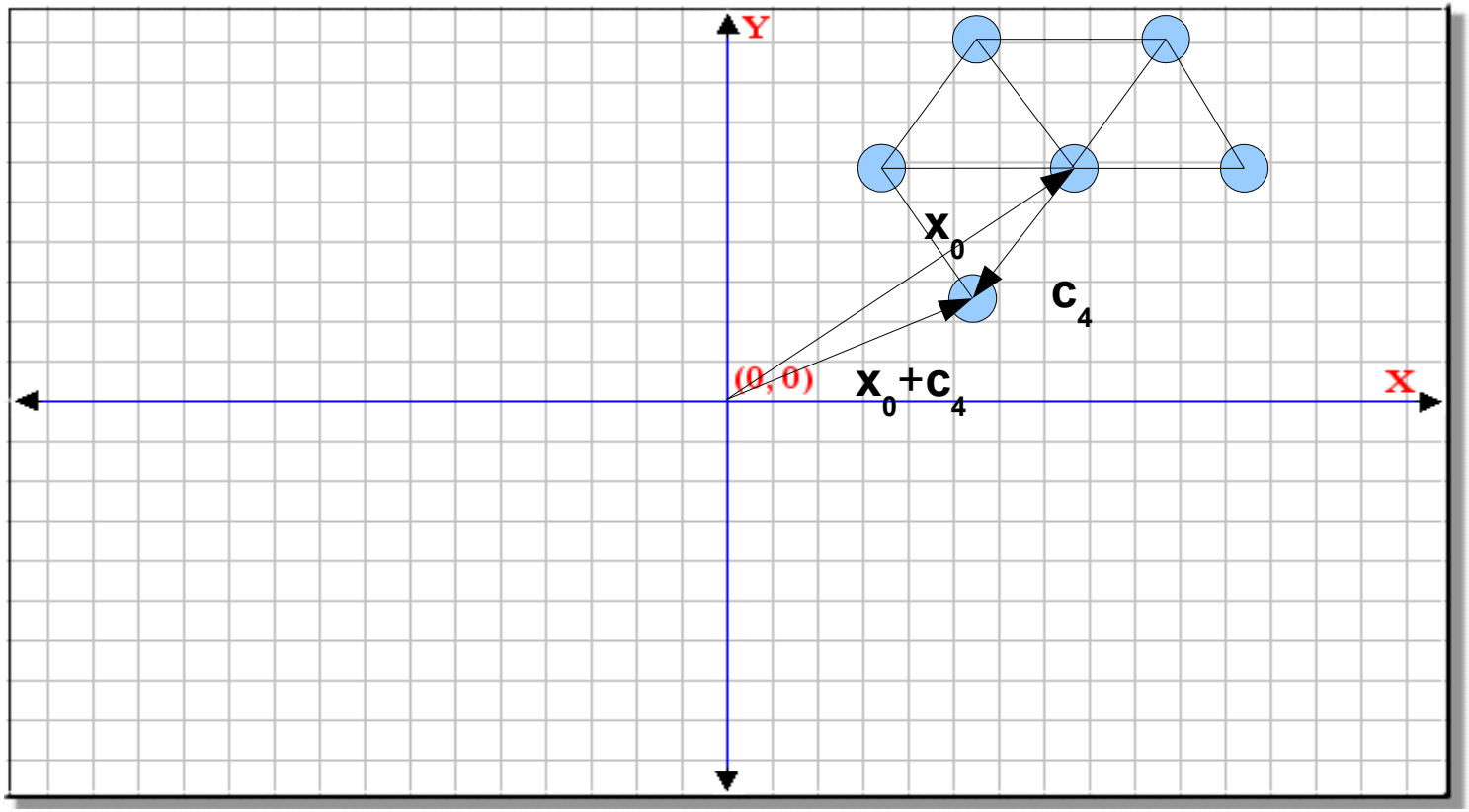
And so on ($x_0 + c_2$)...



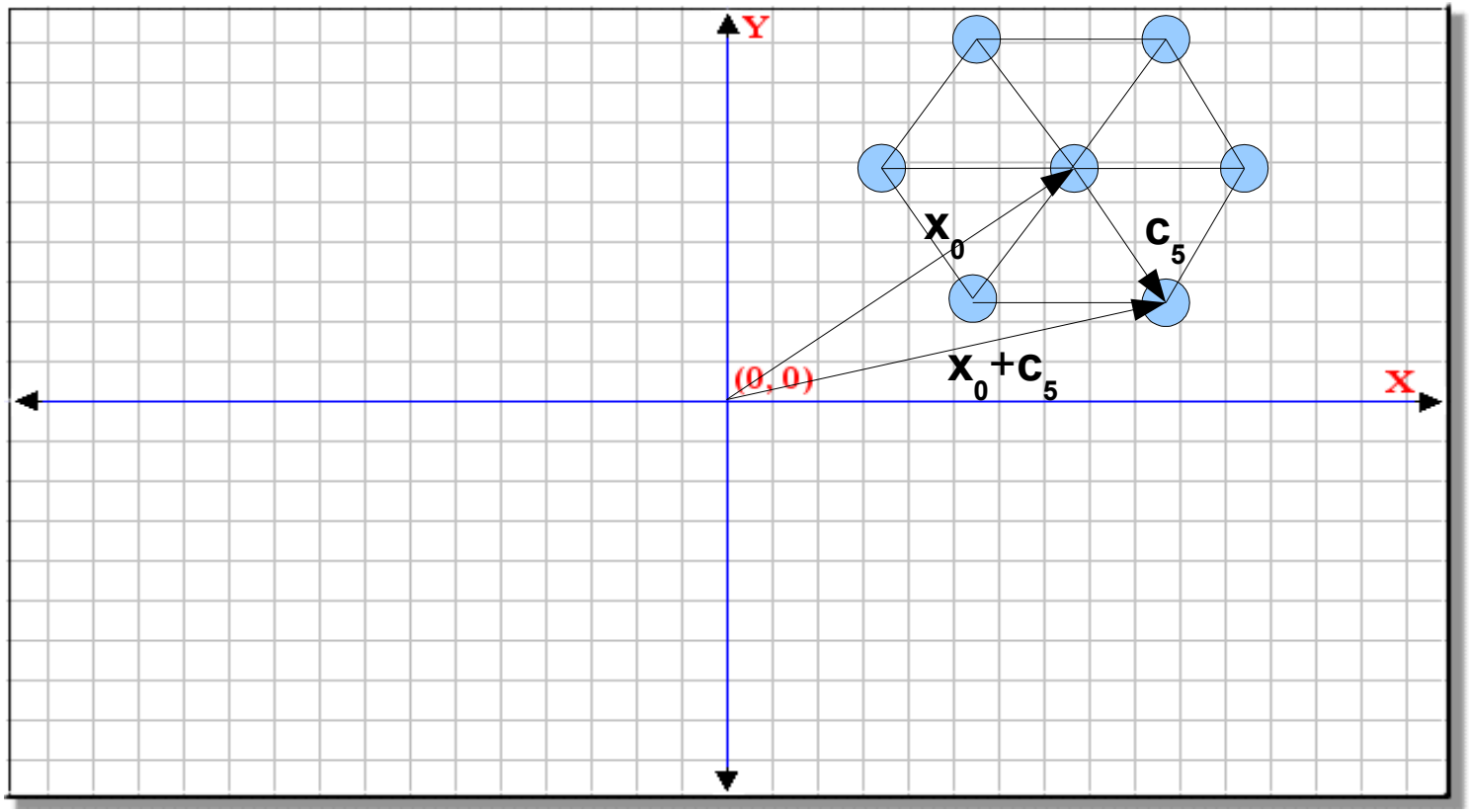
And so on ($x_0 + c_3$)...



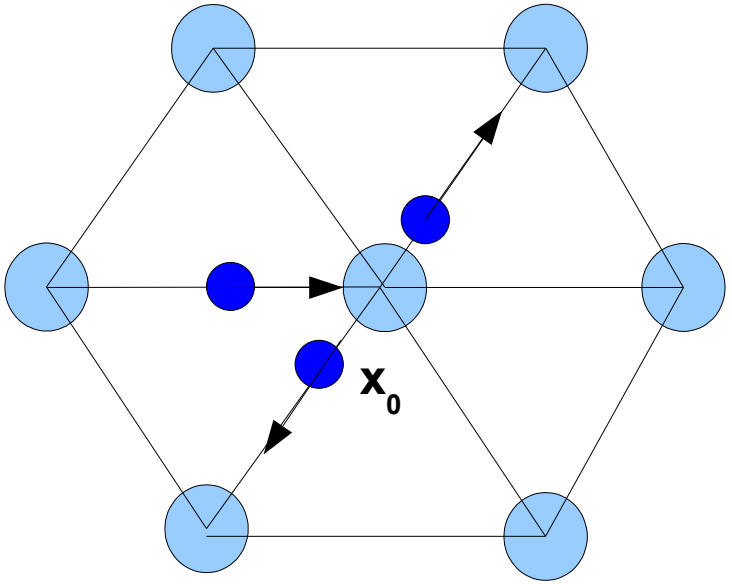
And so on ($x_0 + c_4$)...



And so on ($x_0 + c_5$)...



Denoting particles at a node

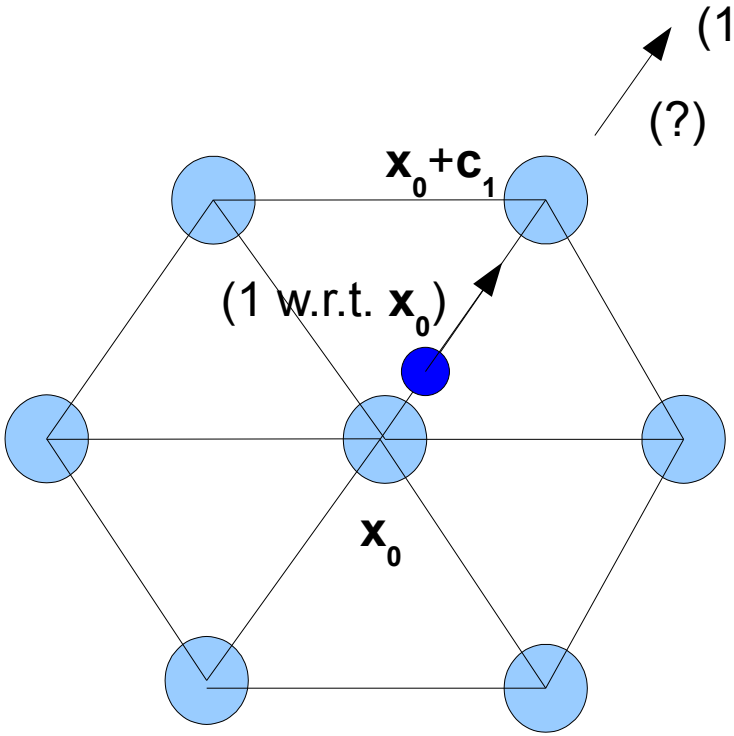


Above:

$n_0(\mathbf{x}_0) = 1;$
$n_1(\mathbf{x}_0) = 1;$
$n_4(\mathbf{x}_0) = 1;$
Others zero.

- Now we have a node at $\mathbf{x}_0$ with all six neighbors.
- We denote the presence of a particle at the node $\mathbf{x}_0$ heading towards the i-th direction with $n_i(\mathbf{x}_0)$
- $n_i(\mathbf{x}_0)$ takes boolean values (0 or 1) depending on the occupancy.

Evolution equation



- $n_i(\mathbf{x}+\mathbf{c}_i,t+1) = n_i(\mathbf{x},t) + \Delta_i[\mathbf{n}(\mathbf{x},t)]$
  - Where $\Delta[\mathbf{n}(\mathbf{x},t)]$ is the "momentum operator" acting on the configuration state $\mathbf{n}(\mathbf{x},t)$.
  - The sophistication of the model depends on the nature of Δ chosen. In my project I deal with only 2- and 3-body collisions.

e.g. Consider i = 1 case:

$n_1(\mathbf{x}+\mathbf{c}_1,t+1) = n_1(\mathbf{x},t) + \Delta_1[\mathbf{n}(\mathbf{x},t)]$

$n_1(\mathbf{x}+\mathbf{c}_1,t+1) = n_1(\mathbf{x},t)$ (Presumably, for the above geometry)

$n_1(\mathbf{x}+\mathbf{c}_1,t+1) = 1$ (i.e. The particle continues on its path.)

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Objectives

- Malleable lattice points; so that I can create the node network “on the fly”
  - This requires some thought into the underlying data structure. The simple two-dimensional array will not suffice for the dynamic network.
- Ability to simulate N>1000 particles at acceptable speeds.
  - This is very modest. (And has been exceeded.) The field picture at the introduction contains time-averaged information on tens of thousands of particles at each arrow.
- Two distinct types of particles.
- Various models of behavior at boundary.

Demo 0:

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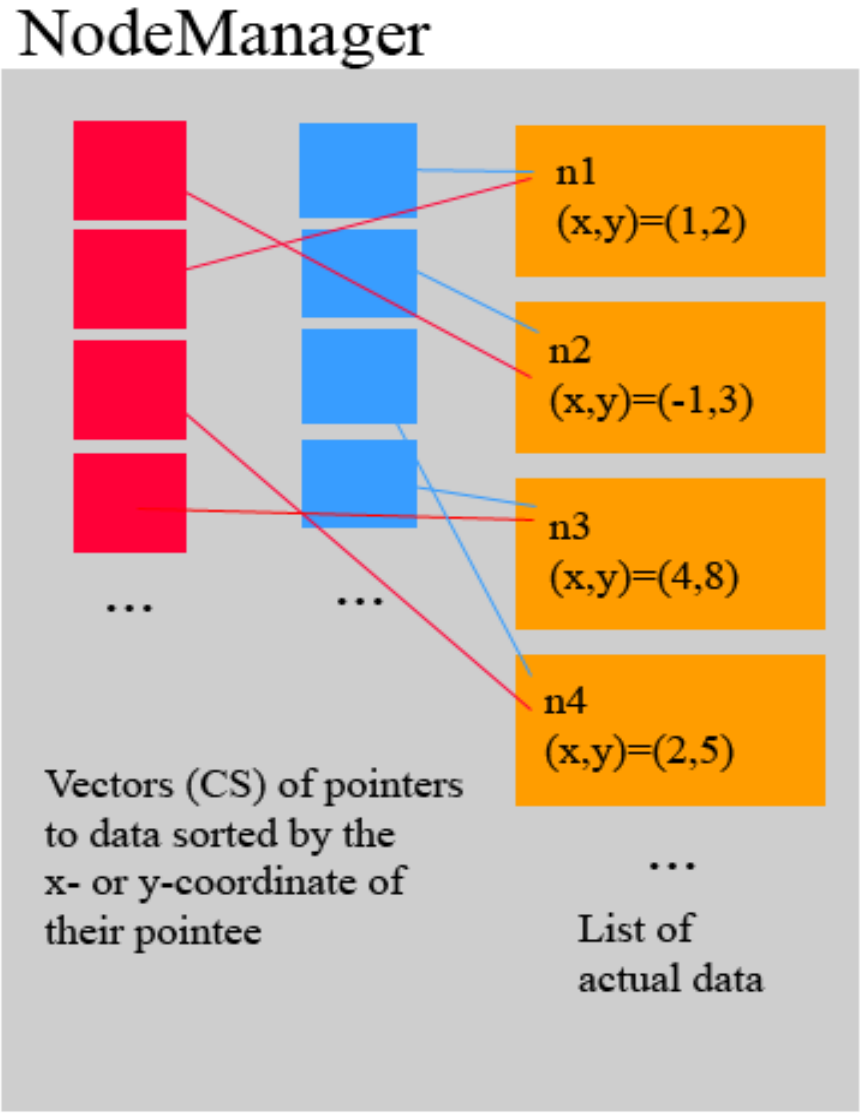
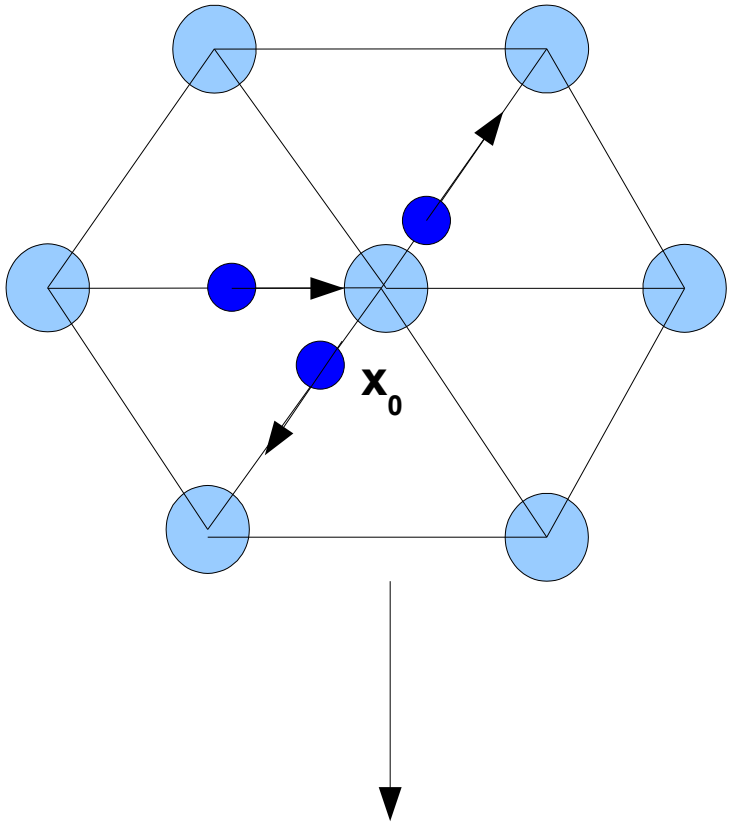
How to manage nodes dynamically

- Dynamic network generation:
  - How does each node – acting very independently – know about and connect to its neighbors?
- How do we achieve this faster than $O(n^2)$, which is why we moved away from the continuous space calculations?
  - Coming up with this solution and its implementation was the most challenging part of this assignment.



Computing collisions faster: Boolean operations at the bit level

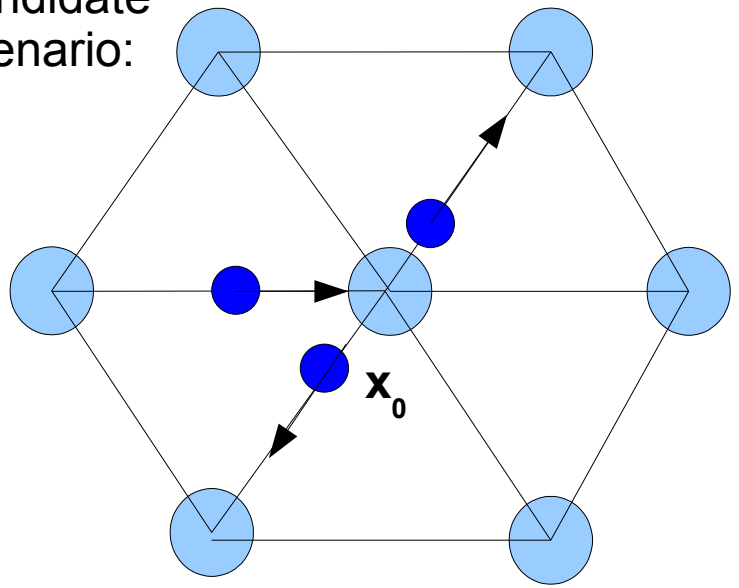


x	x	0	1	0	0	1	1
7	6	5	4	3	2	1	0

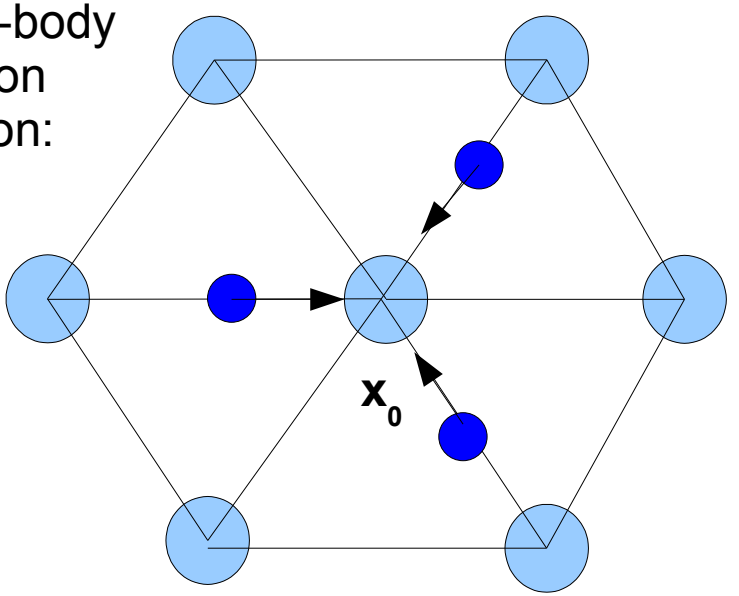
- Take advantage of the fact that occupancy is represented by a boolean variable (0 or 1).
- Represent occupancy by using 6-bits of a byte.

Example: Detecting a three-body head-on collision via bit operations

Candidate Scenario:



Three-body head-on collision:



x	x	0	1	0	0	1	1
7	6	5	4	3	2	1	0

x	x	0	1	0	1	0	1
7	6	5	4	3	2	1	0

Does the scenario on the left correspond to a three-body head-on collision?

Three-body head-on collision

Actual configuration:

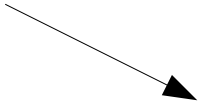
x	x	0	1	0	0	1	1
7	6	5	4	3	2	1	0

Heads-on three-body collision state:

x	x	0	1	0	1	0	1
7	6	5	4	3	2	1	0

Bitwise AND (&):

x	x	0	1	0	0	0	1
7	6	5	4	3	2	1	0



No match!

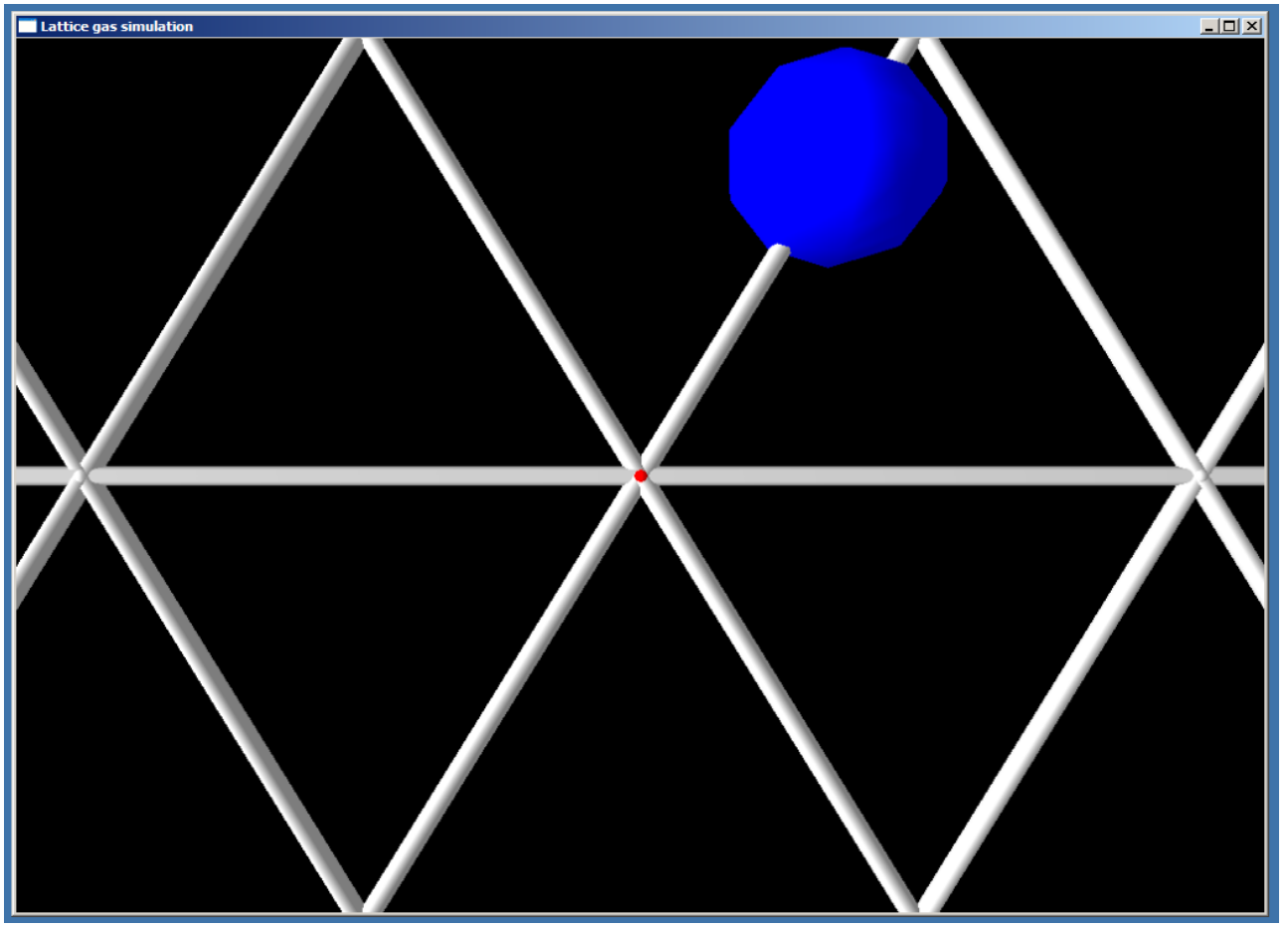
We do NOT have the particular three-body collision.

1) "Mask" (bitwise AND) the actual configuration with the candidate scenario;
2) Bitwise comparison of the masked result to the candidate scenario.
3) If equivalent, then we have a three-body head-on collision as shown.

Huge advantage over continuous simulations

- Calculation of a *three-body collision* has been reduced to two primitive operations:
  - Masking;
  - Equality checking;
- Furthermore, the number of calculations per frame is NOT dependent on particle number!
  - Instead, it depends on the number of *nodes;*
  - The number of computations increases only **linearly** with the number of nodes, once the network is configured!

So what do we do with the “extra” processing power?



- Squander it on rendering**!**

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