Advanced Monte Carlo algorithms

Bad Honnef Physics School
Computational Physics of Complex and Disordered Systemss

Werner Krauth

Département de Physique
Ecole Normale Supérieure, Paris, France

23 September 2015

- Monte Carlo algorithms - basic notions.
- Hard disks: From detailed balance to global balance and to cluster algorithms.
- Integration and Sampling: From Gaussians to Maxwell and Boltzmann.
- Cluster algorithms for spin models: Ising, XY, Spin glasses.

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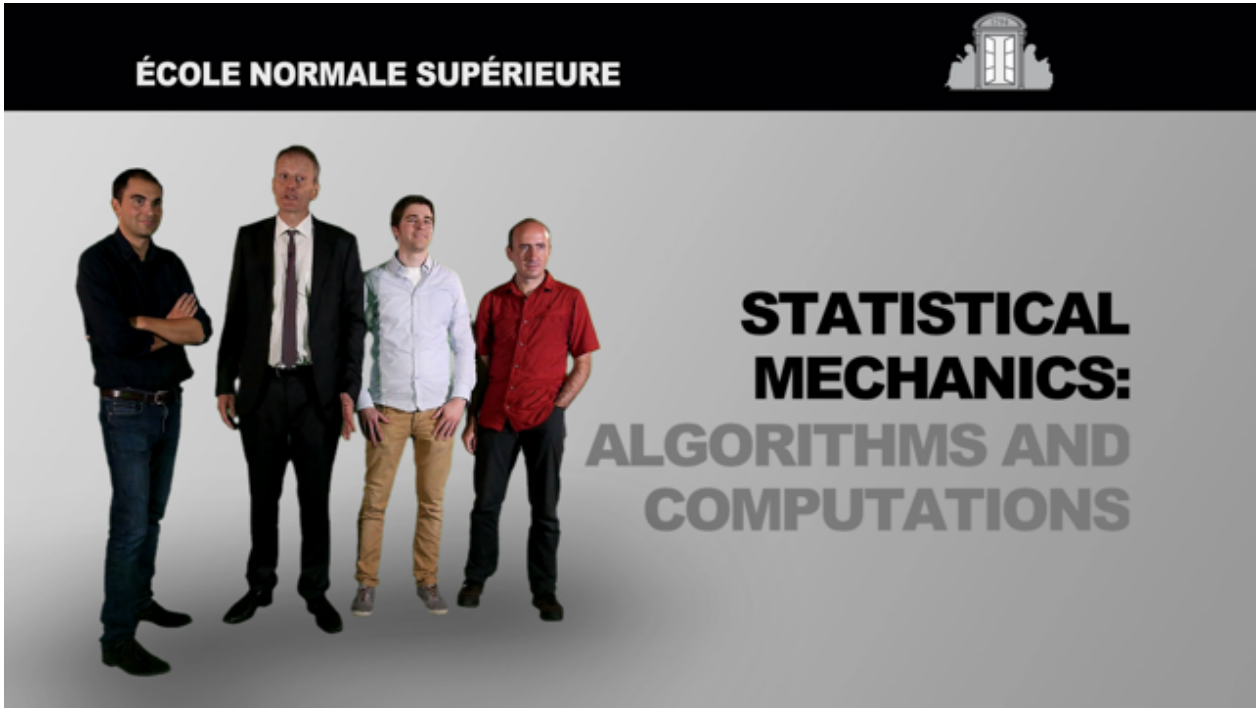
MOOC Statistical Mechanics: Algorithms and Computations



- see also: Werner Krauth *Statistical Mechanics: Algorithms and Computations* (Oxford, 2006)

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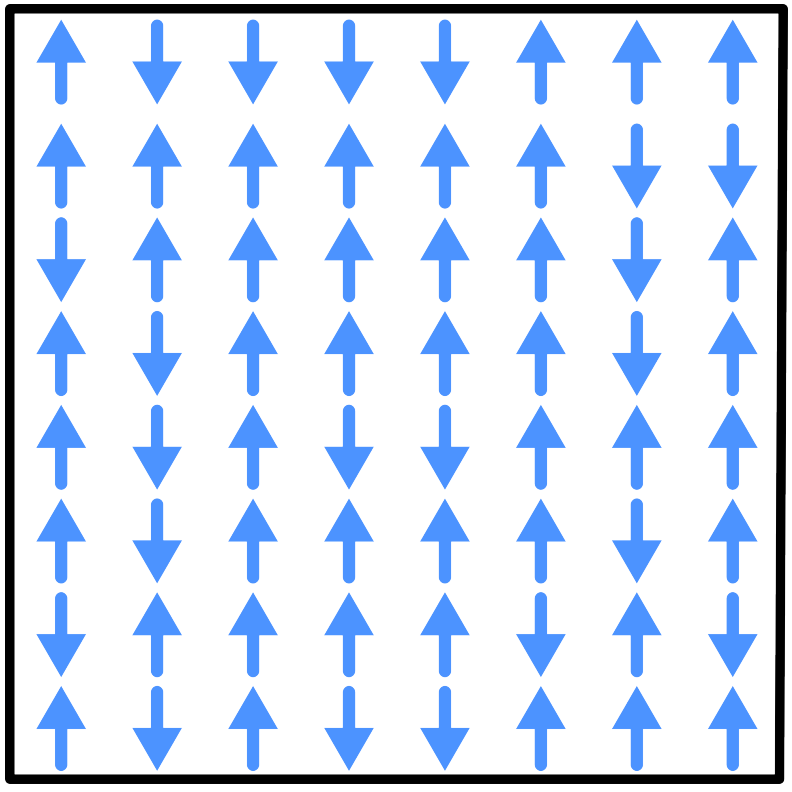
Ising model



- spins $\sigma = \pm 1$

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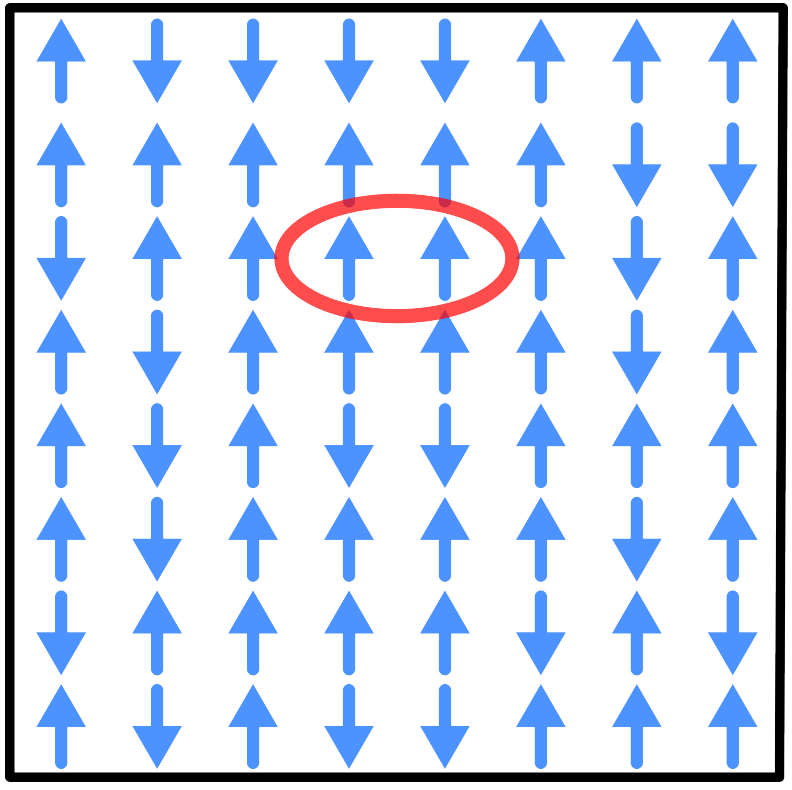
Ising model



- pair energy $E_{ij} = -1$

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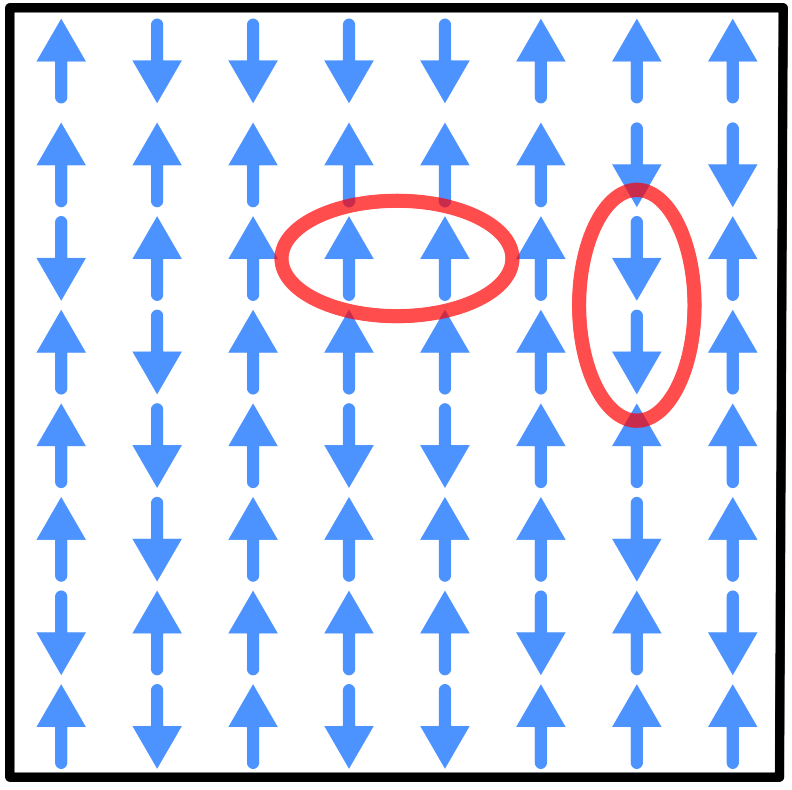

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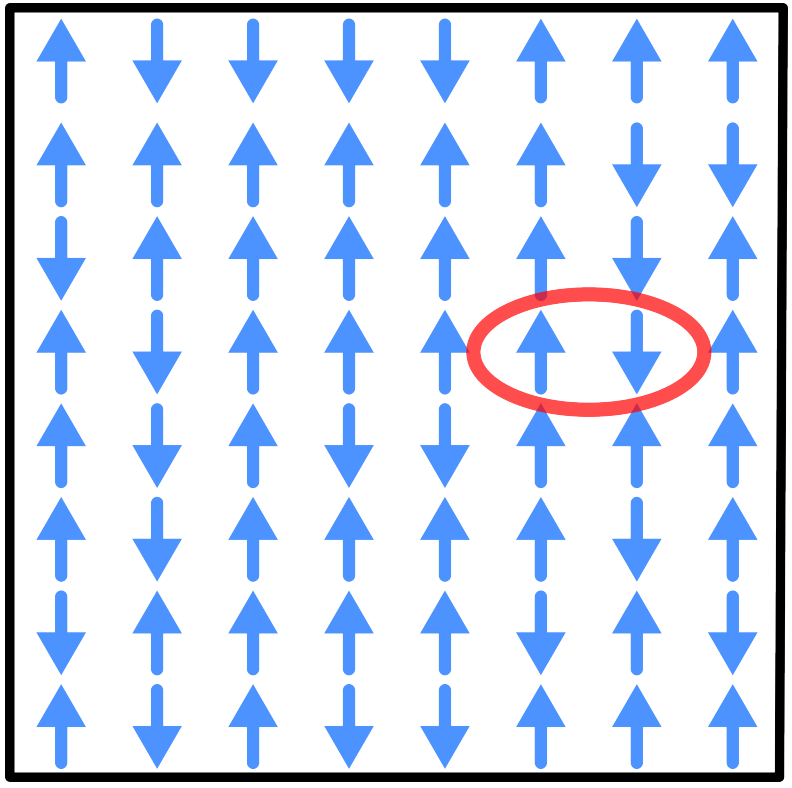
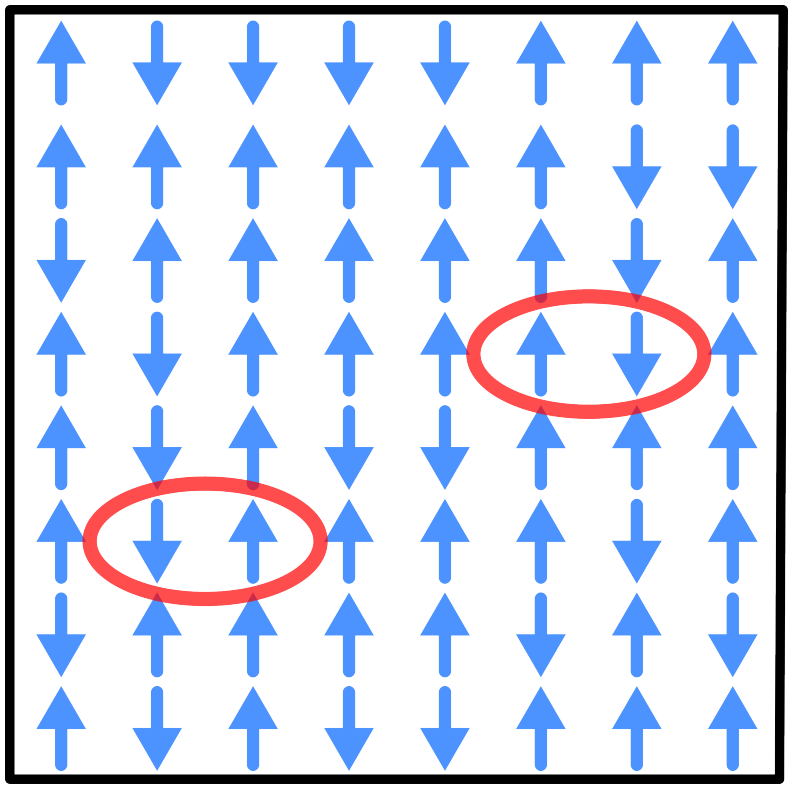


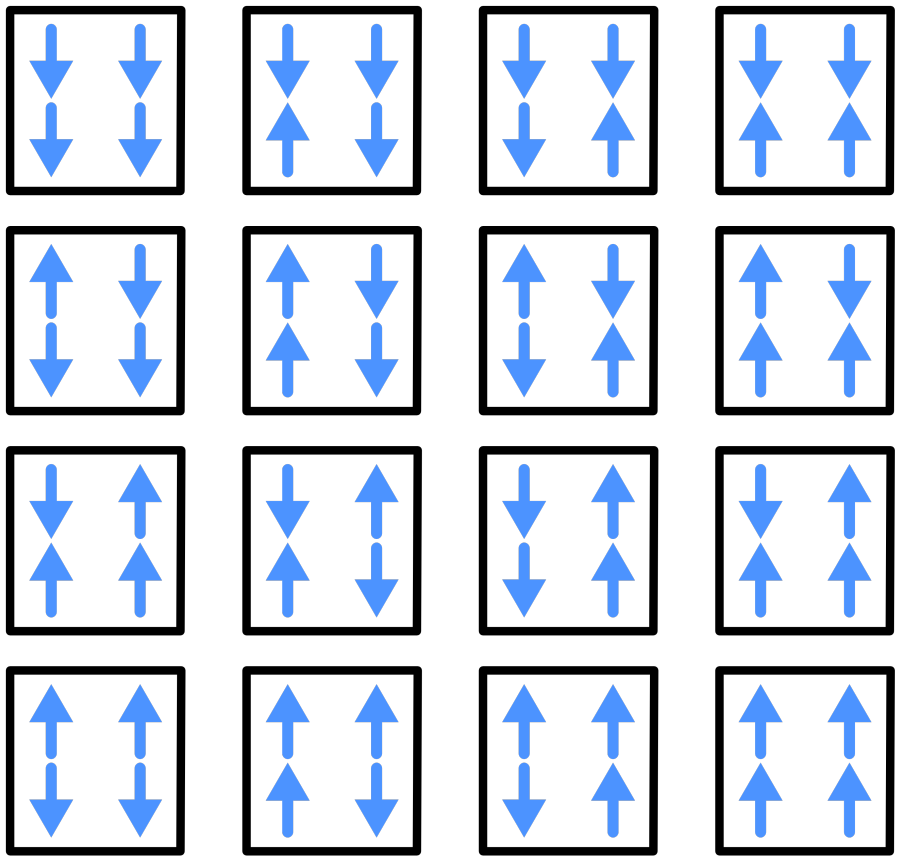
- pair energy $E_{ij} = +1$

Ising model

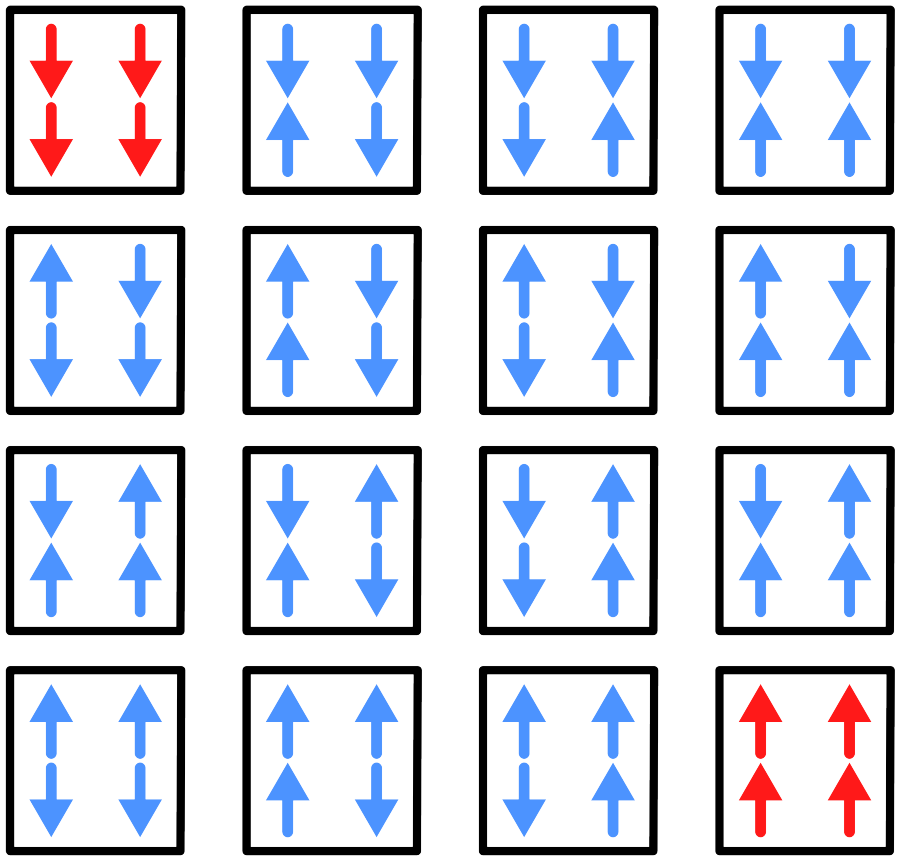


- pair energies $E_{ij} = +1$

2x2 Ising model



2x2 Ising model



E=-4

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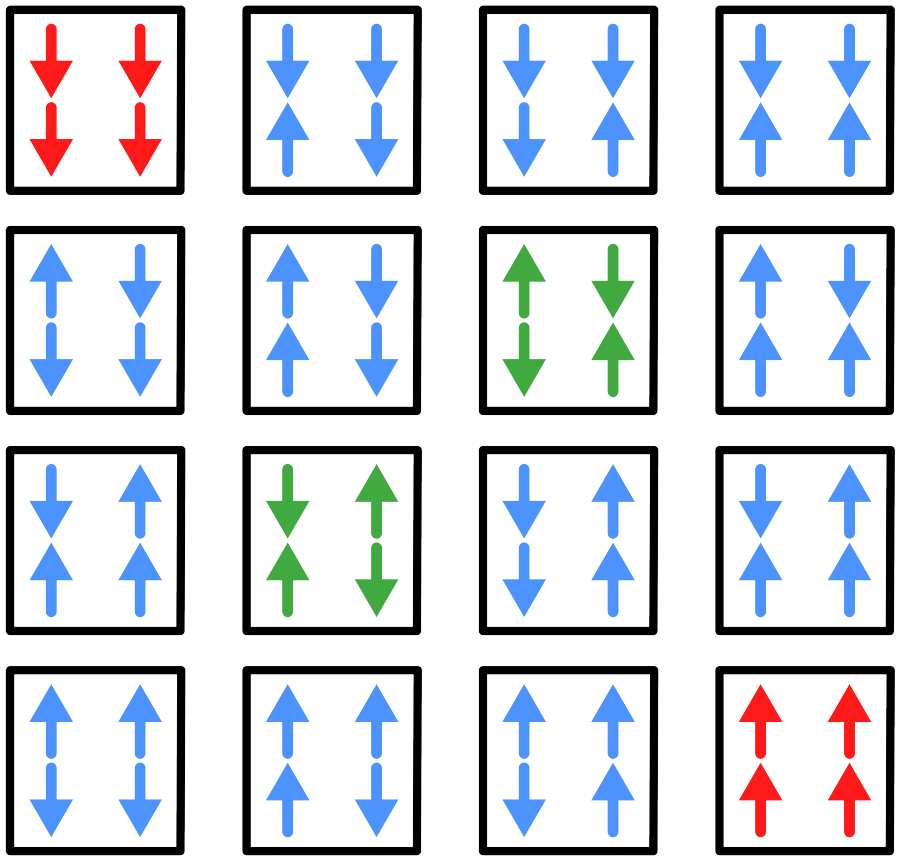
2x2 Ising model



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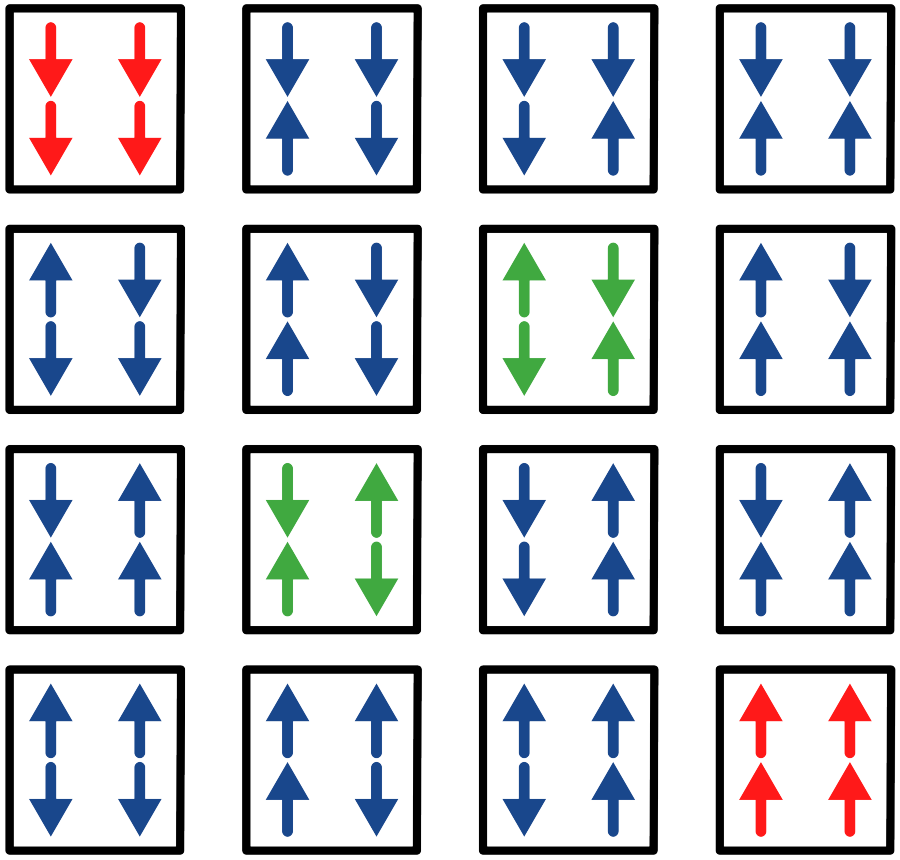

E=-4 E=4 E=0

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Gray-code enumeration

```
[-1, -1, -1, -1]  E = -4
```

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[-1, -1, -1,  1]  E =  0
```

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enumerate-ising.py

```
def gray_flip(t, N):
    k = t[0]
    if k > N: return t, k
    t[k - 1] = t[k]
    t[k] = k + 1
    if k != 1: t[0] = 1
    return t, k

L = 4
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N)
                                        for i in range(N)}
S = [-1] * N
E = -2 * N
print S, E
tau = range(1, N + 2)
for i in range(1, 2 ** N):
    tau, k = gray_flip(tau, N)
    h = sum(S[n] for n in nbr[k - 1])
    E += 2 * h * S[k - 1]
    S[k - 1] *= -1
    print S, E
```

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Partition function

$$Z(\beta) = - \sum_{\substack{\sigma_0 = \pm 1 \\ \dots \\ \sigma_{N-1} = \pm 1}} e^{-\beta E(\sigma_0, \dots, \sigma_{N-1})}$$

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$$= \sum_E \mathcal{N}(E) e^{-\beta E}$$

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Computation of observables

$$\langle E \rangle = \frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}} \, e^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}} e^{-\beta E_{\boldsymbol{\sigma}}}}$$

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Computation of observables

$$\langle E \rangle = \frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}} \, e^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}} e^{-\beta E_{\boldsymbol{\sigma}}}}$$

$$= \sum_{E} E \, \mathcal{N}(E) \, e^{-\beta E}$$

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thermo-ising.py

```
L = 4
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N) \
                                        for i in range(N)}
dos = {}
S = [-1] * N
E = energy(S, N, nbr)
dos[E] = 1
tau = range(1, N + 2)
for i in range(1, 2 ** N):
    tau, k = gray_flip(tau, N)
    E += 2 * sum(S[k - 1] * S[n] for n in nbr[k - 1])
    S[k - 1] *= -1
    if E in dos: dos[E] += 1
    else:        dos[E] = 1
for T in [0.1 * i for i in range(1, 51)]:
    Z = 0.0
    E_av = 0.0
    M_av = 0.0
    E2_av = 0.0
    for E in dos.keys():
        weight = math.exp(- E / T) * dos[E]
        Z += weight
        E_av += weight * E
        E2_av += weight * E ** 2
    E2_av /= Z
    E_av /= Z
    cv = (E2_av - E_av ** 2) / N / T
```

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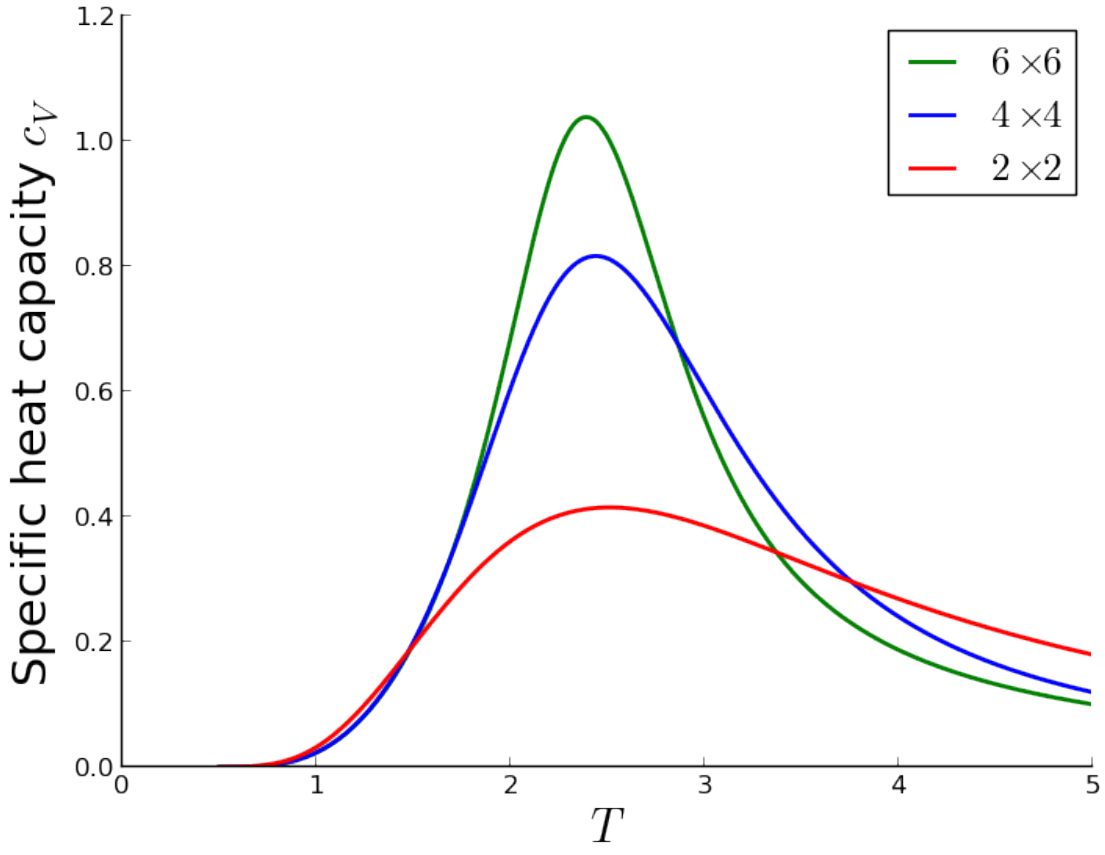
Specific heat of Ising model on finite lattices



$$T_c = \frac{2}{\log(1+\sqrt{2})} = 2.269...$$

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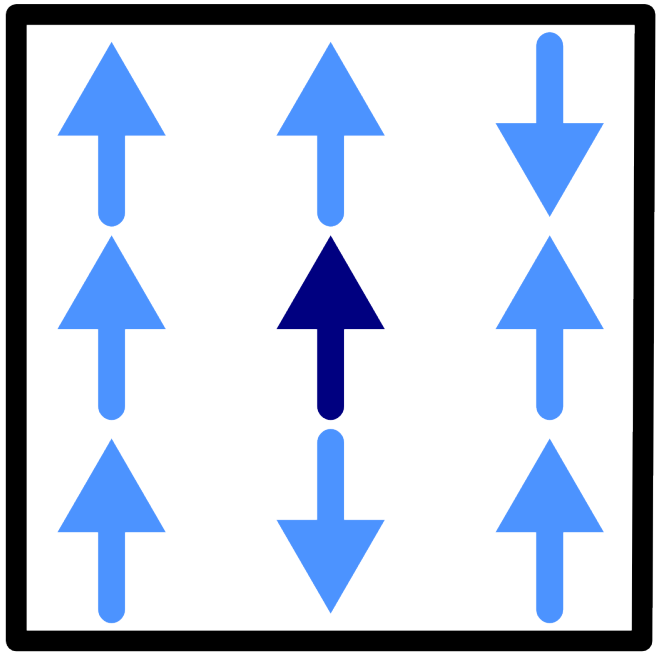
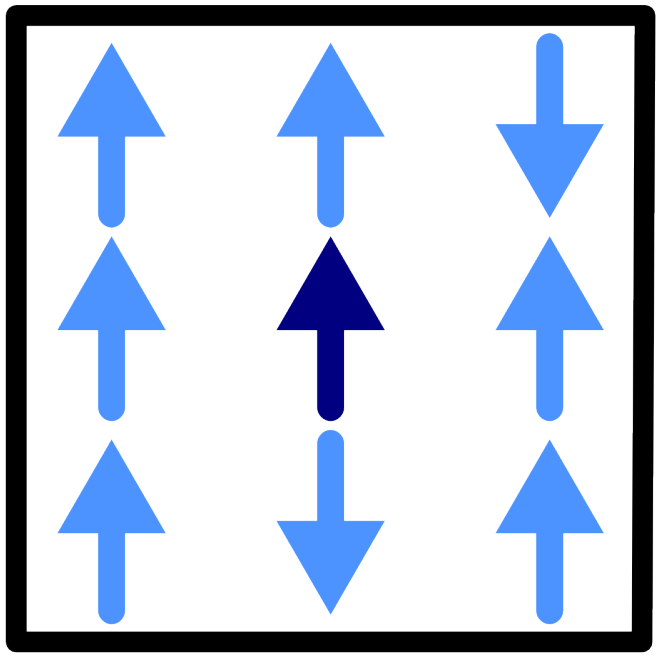
Markov-chain sampling



Markov-chain sampling



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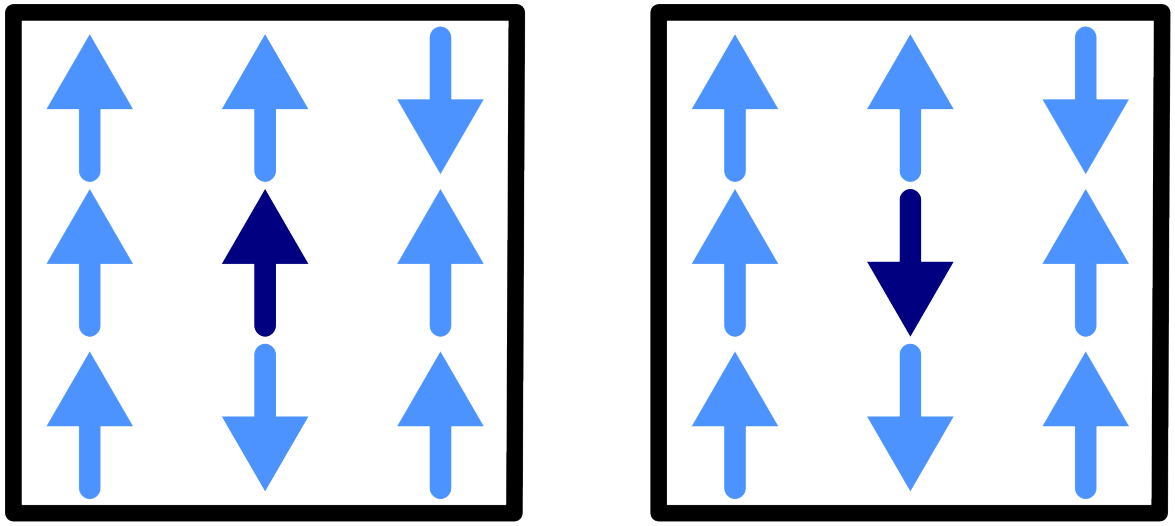
Markov-chain sampling



$$p^{\mathrm{acc}}(a \to b) = \min\left(1, e^{-\beta(E_b - E_a)}\right)$$

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markov-ising.py

```
import random, math

L = 16
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N) \
                                        for i in range(N)}
nsteps = 1000000
T = 2.0
beta = 1.0 / T
S = [random.choice([1, -1]) for k in range(N)]
for step in range(nsteps):
    k = random.randint(0, N - 1)
    delta_E = 2.0 * S[k] * sum(S[nn] for nn in nbr[k])
    if random.uniform(0.0, 1.0) < math.exp(-beta * delta_E):
        S[k] *= -1
print S, sum(S)
```

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Configurations around Tc

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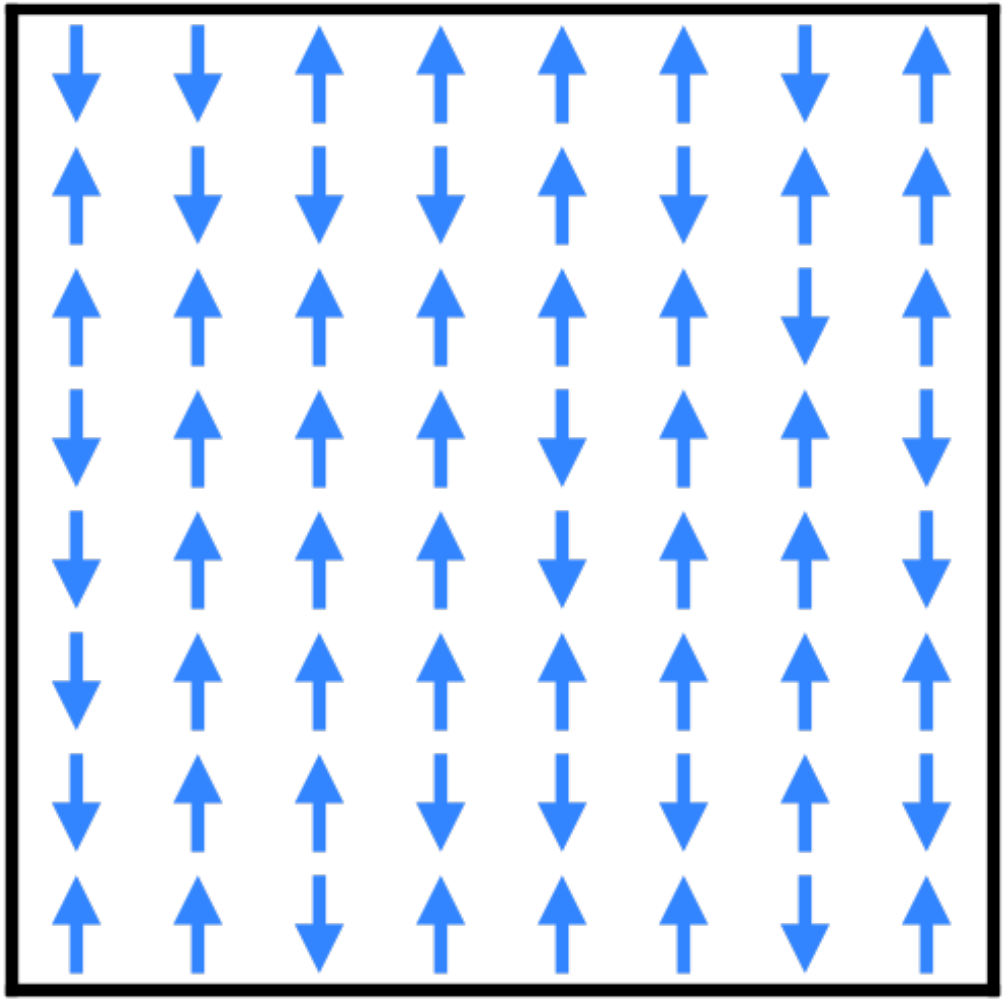
Cluster algorithm, first idea



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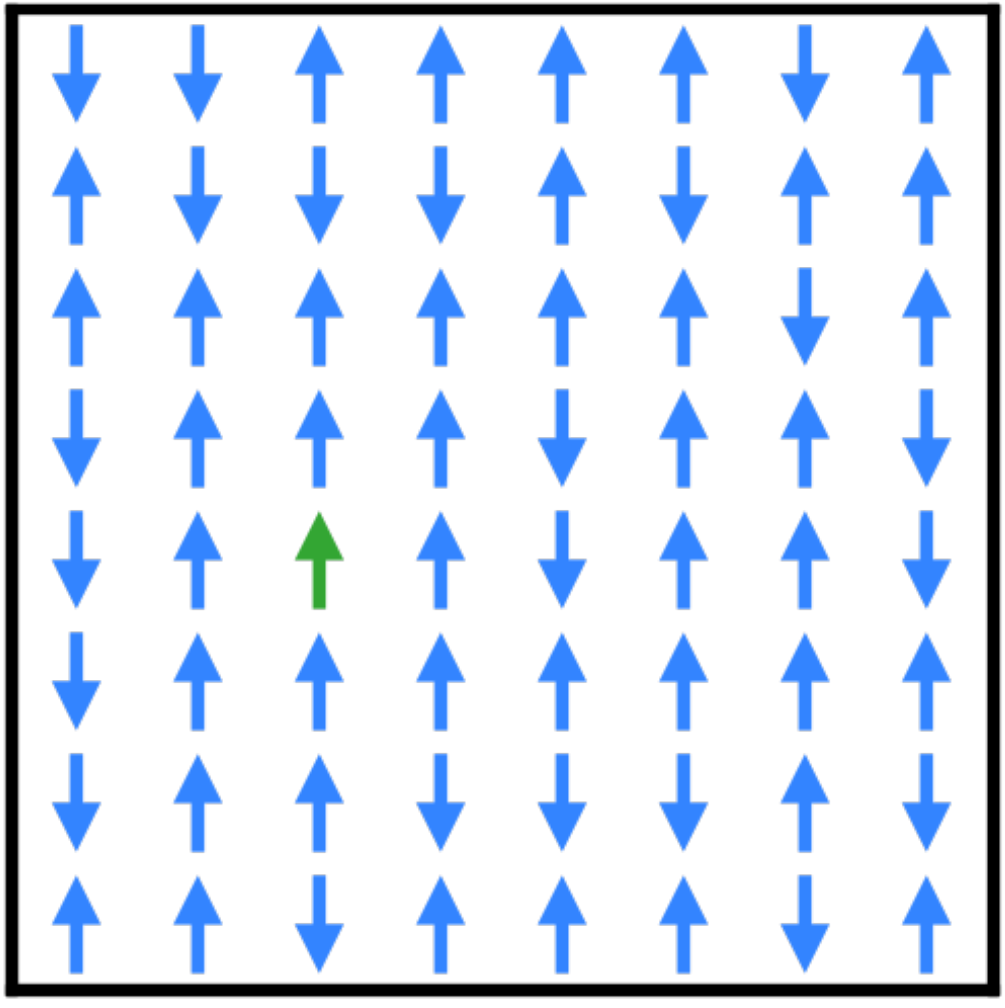

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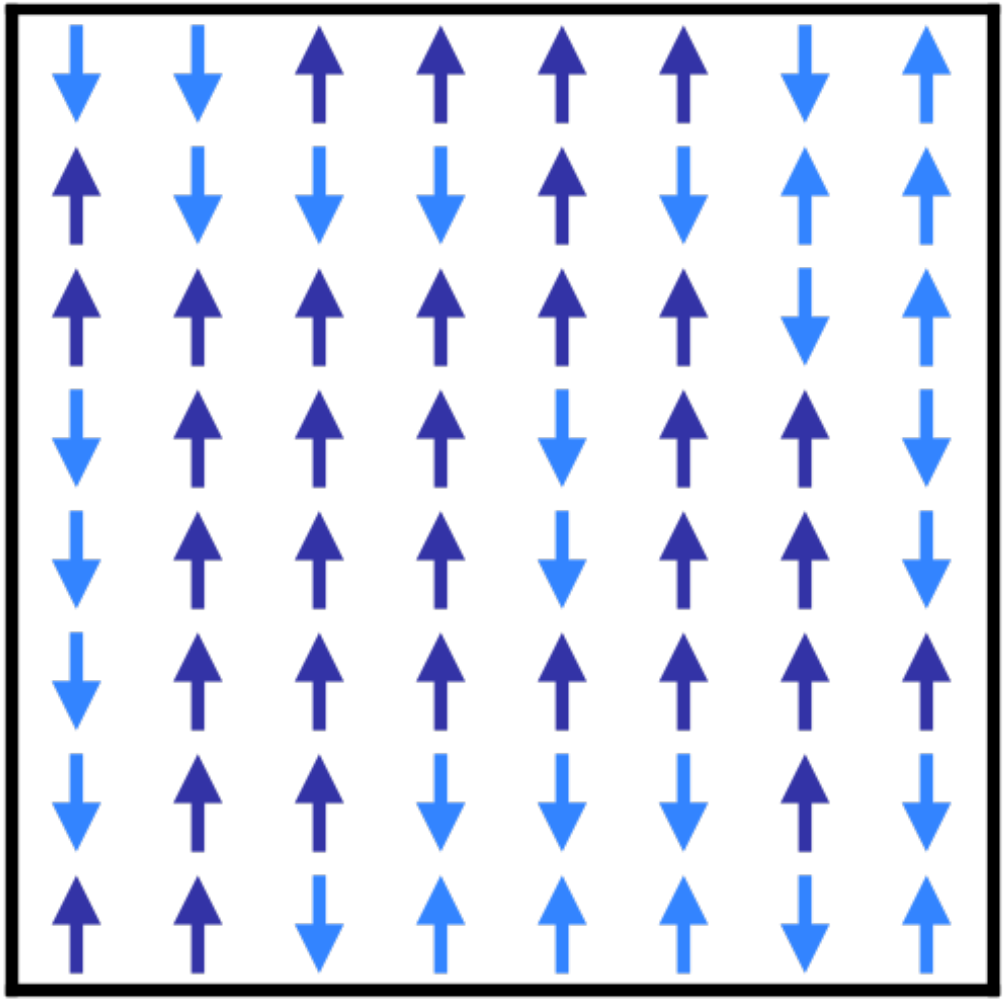

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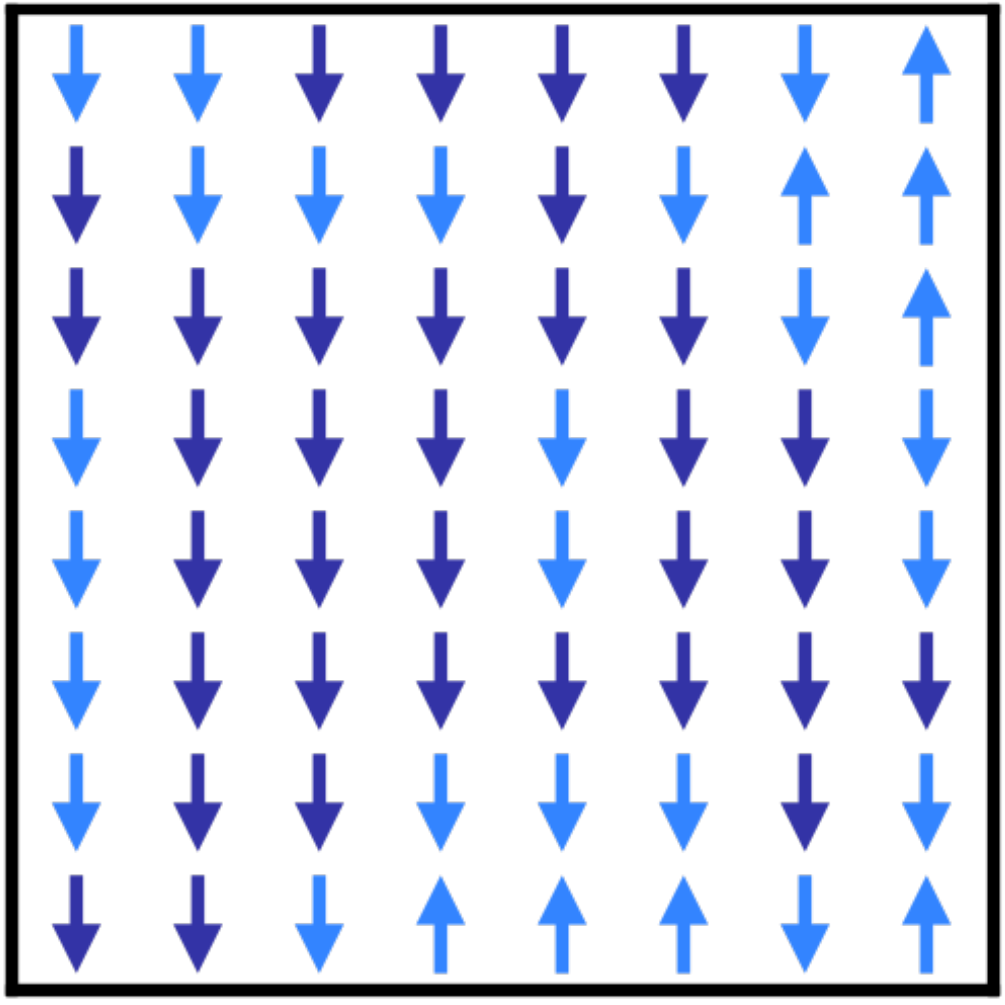

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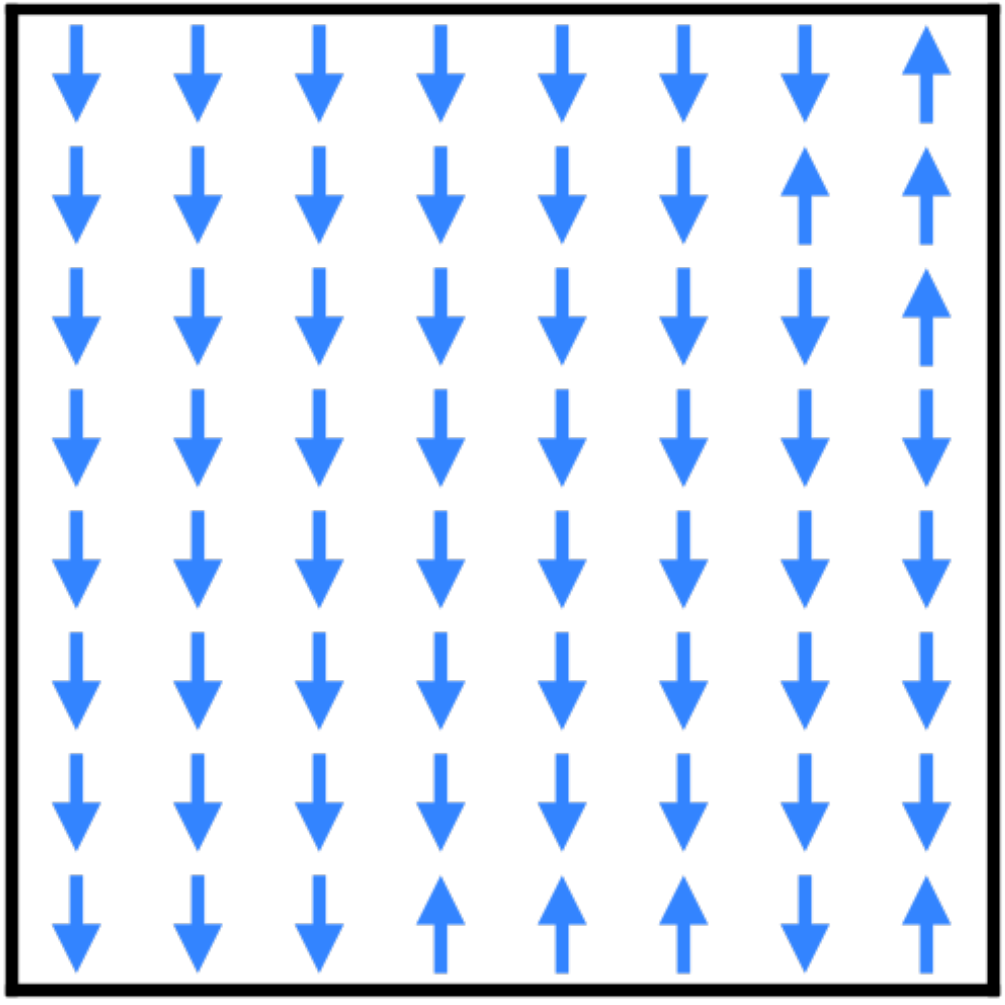

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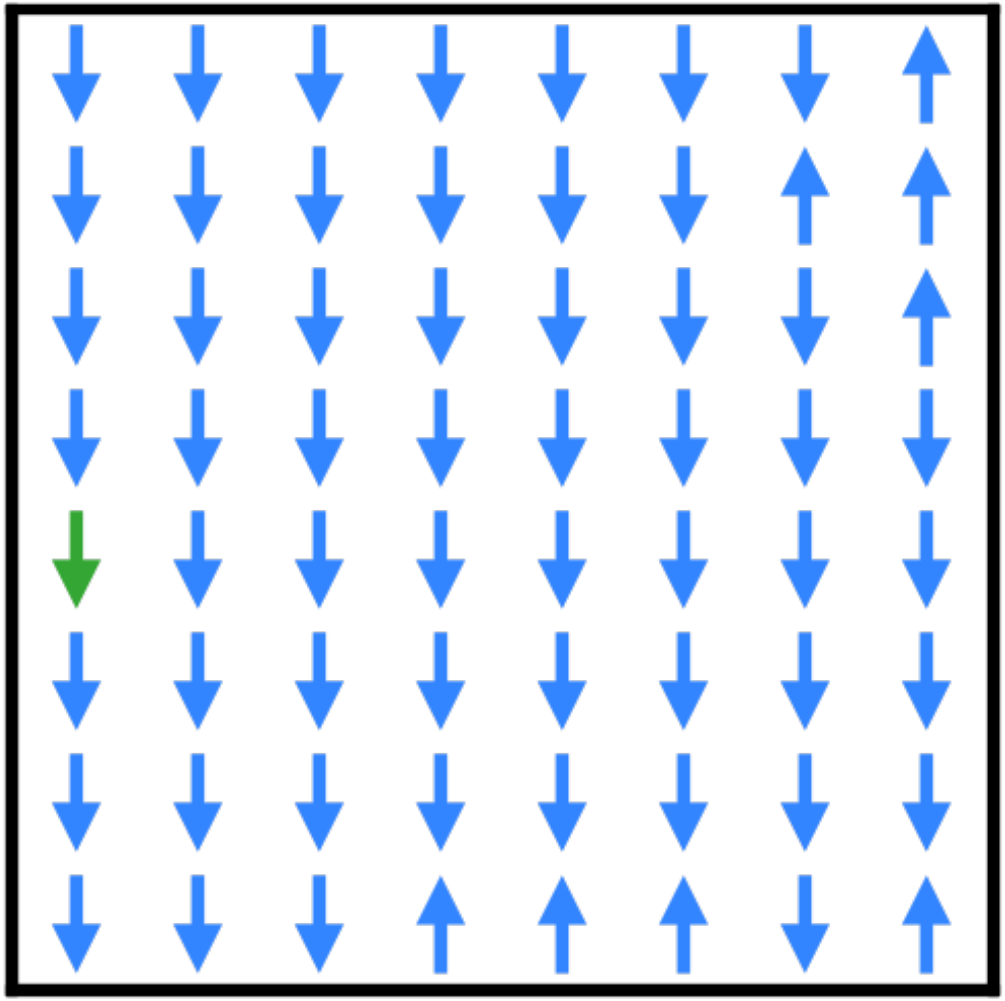

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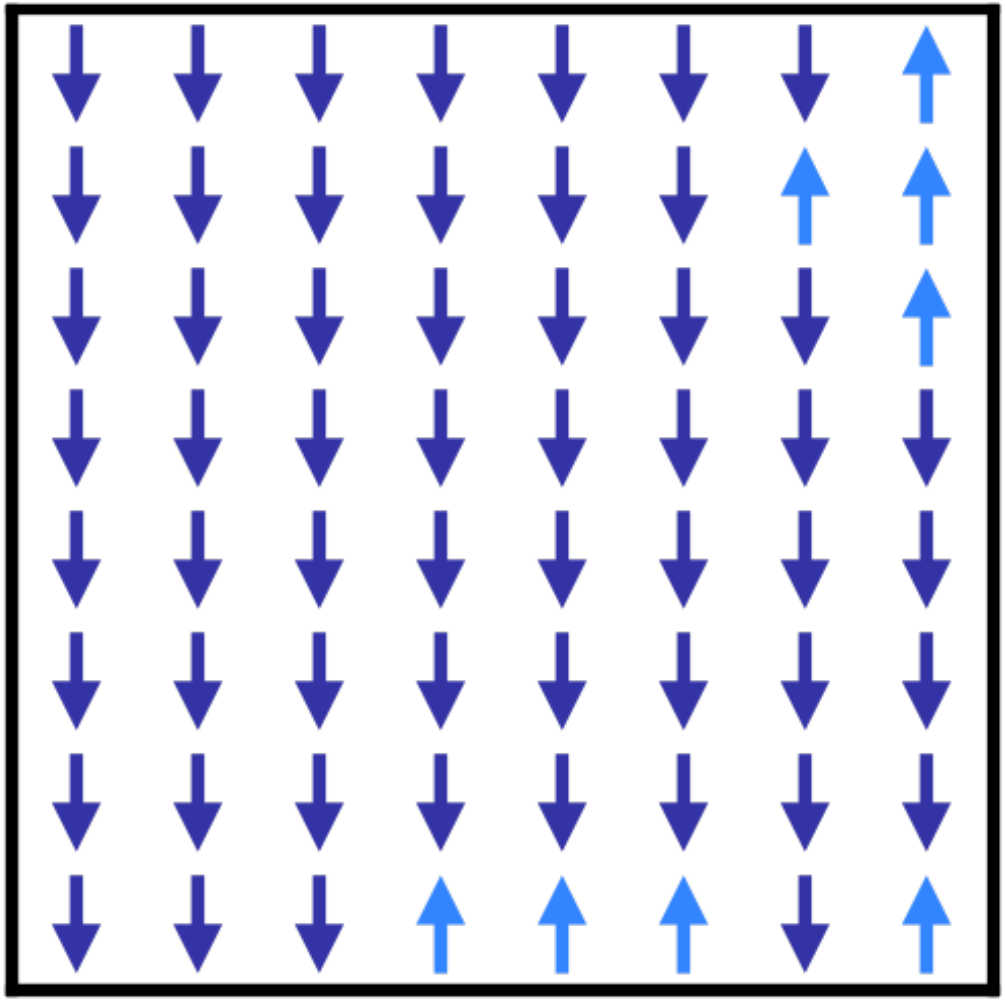

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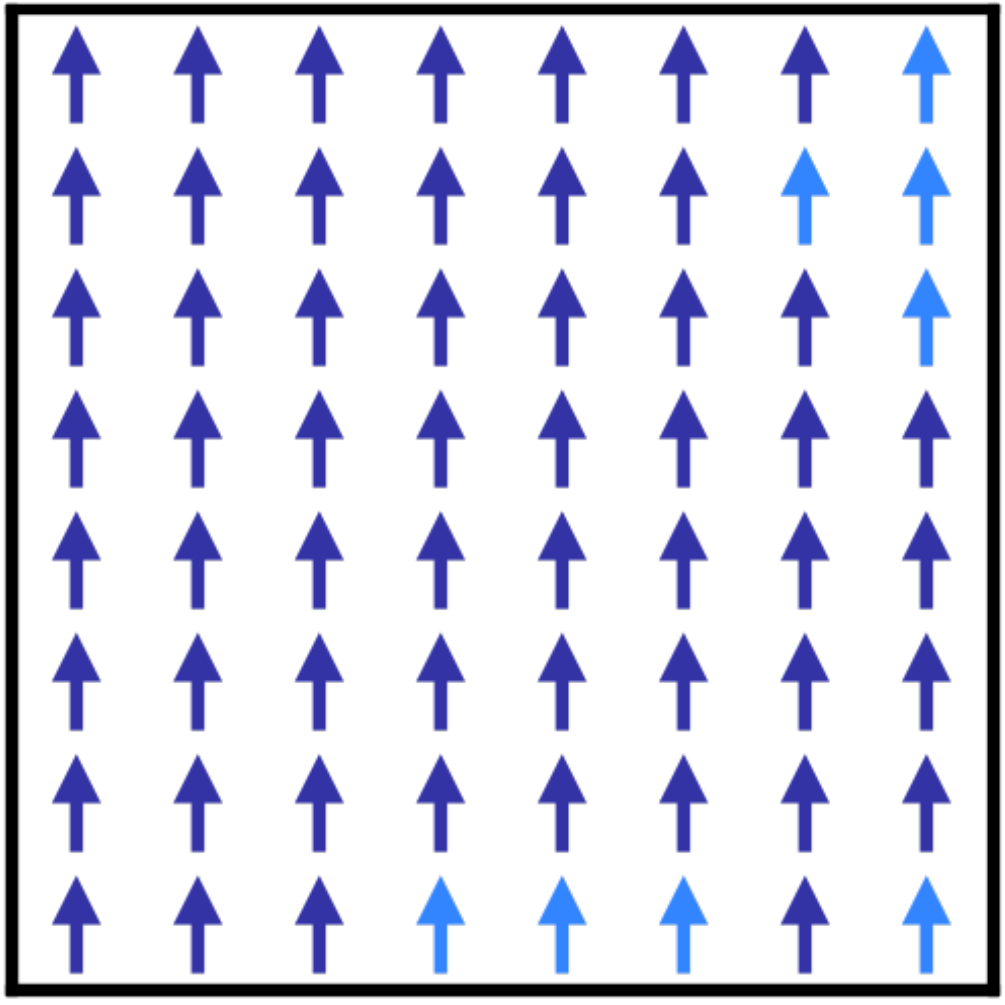
Cluster algorithm, first idea



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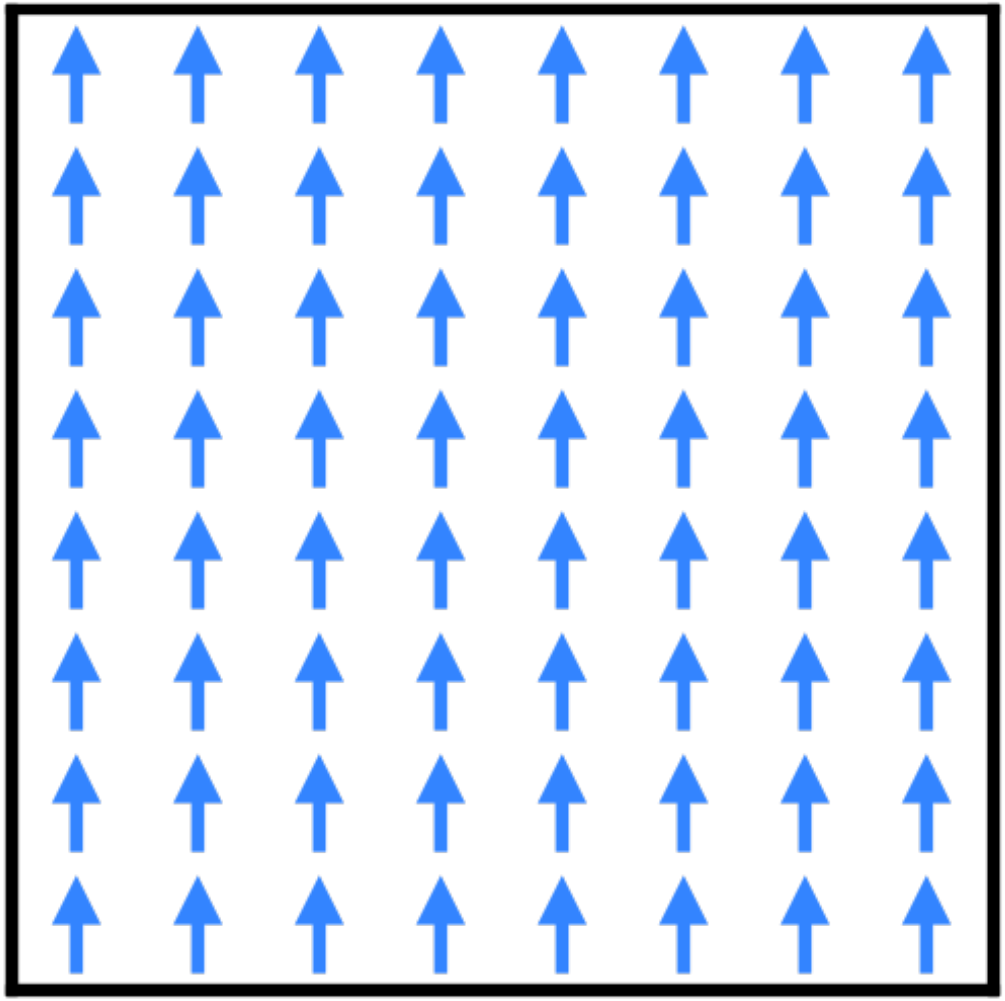

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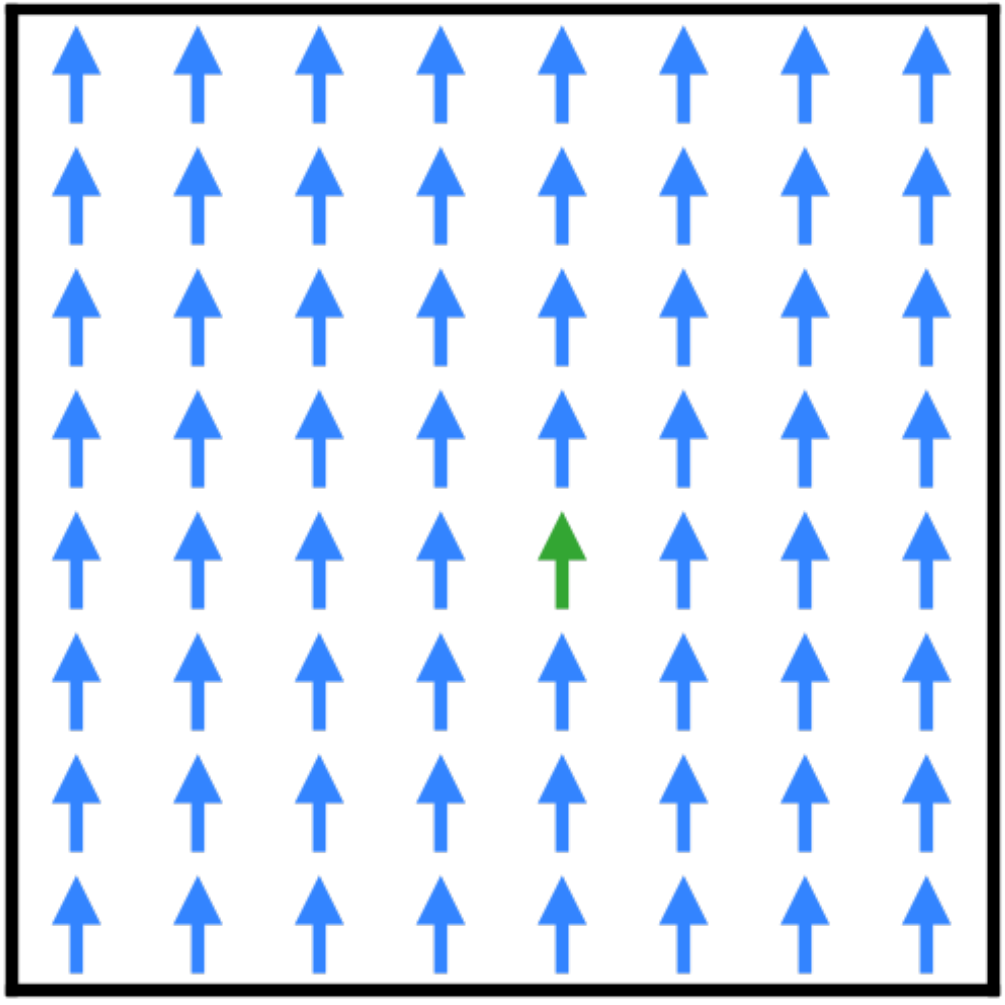

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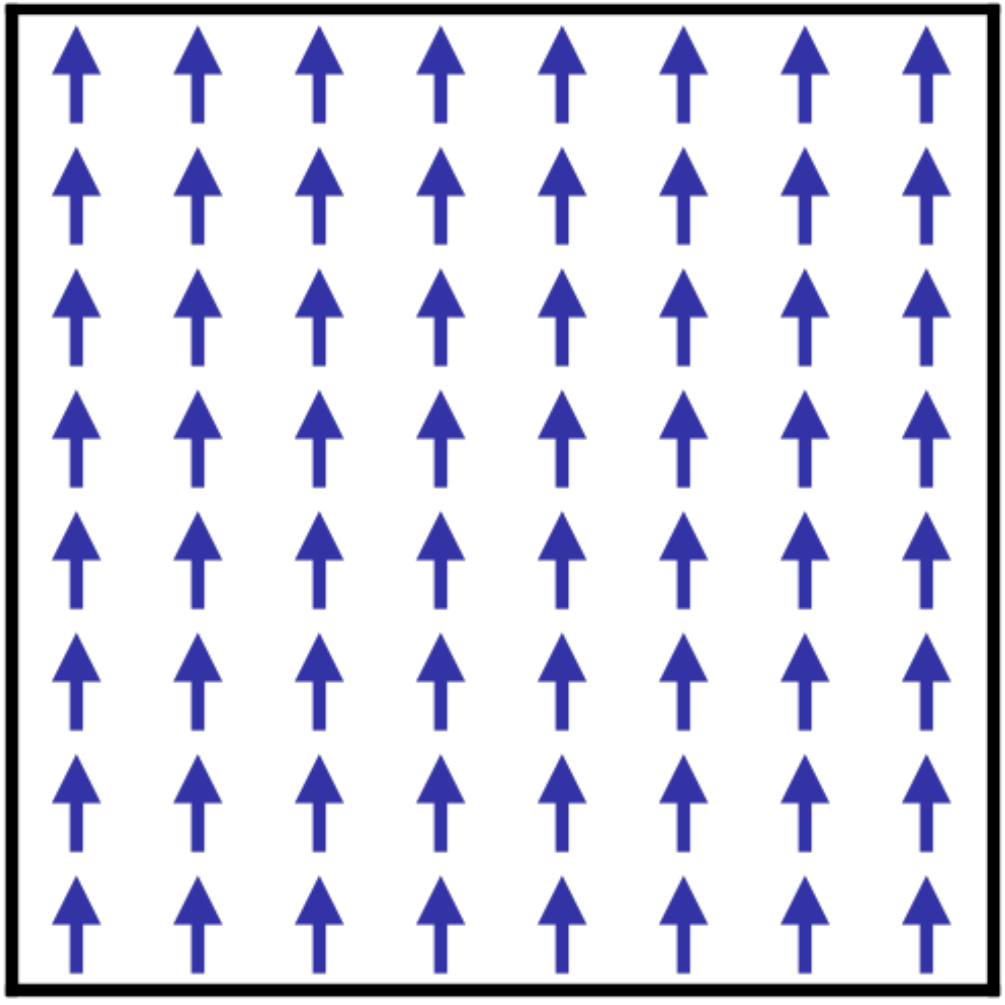

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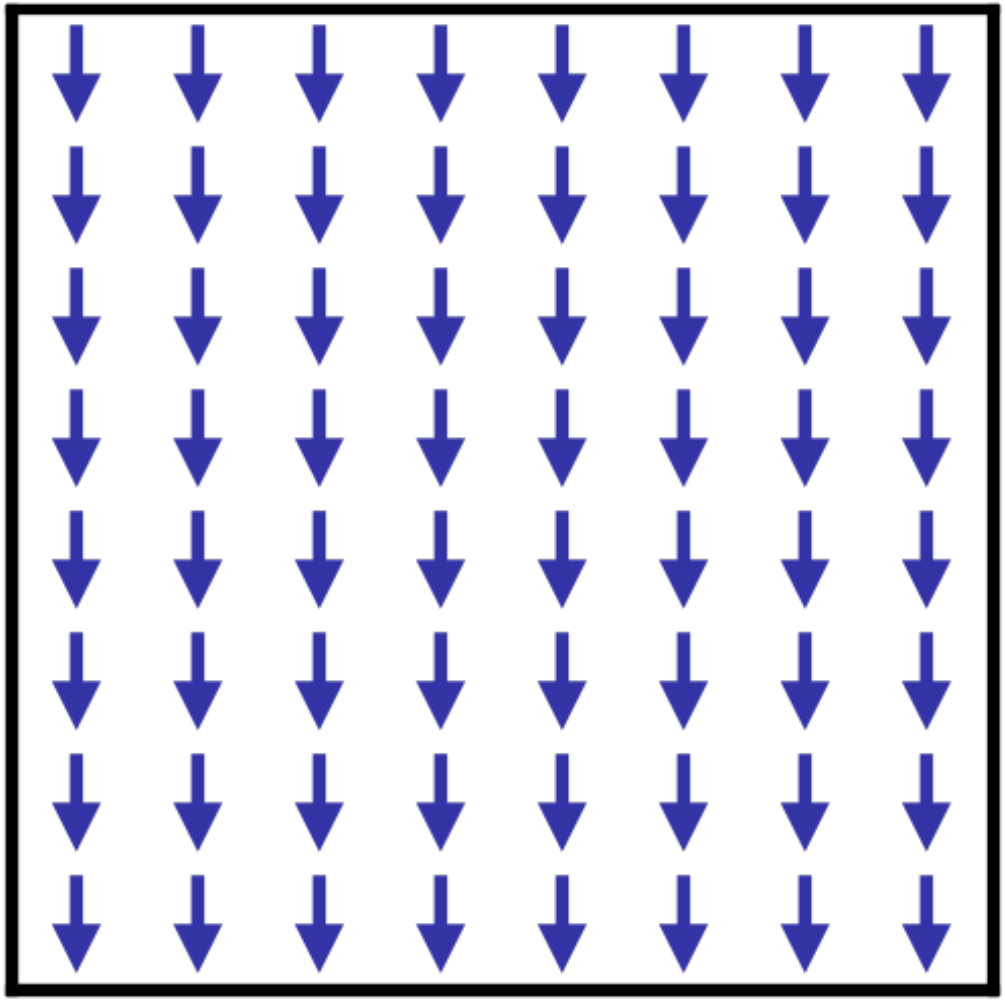

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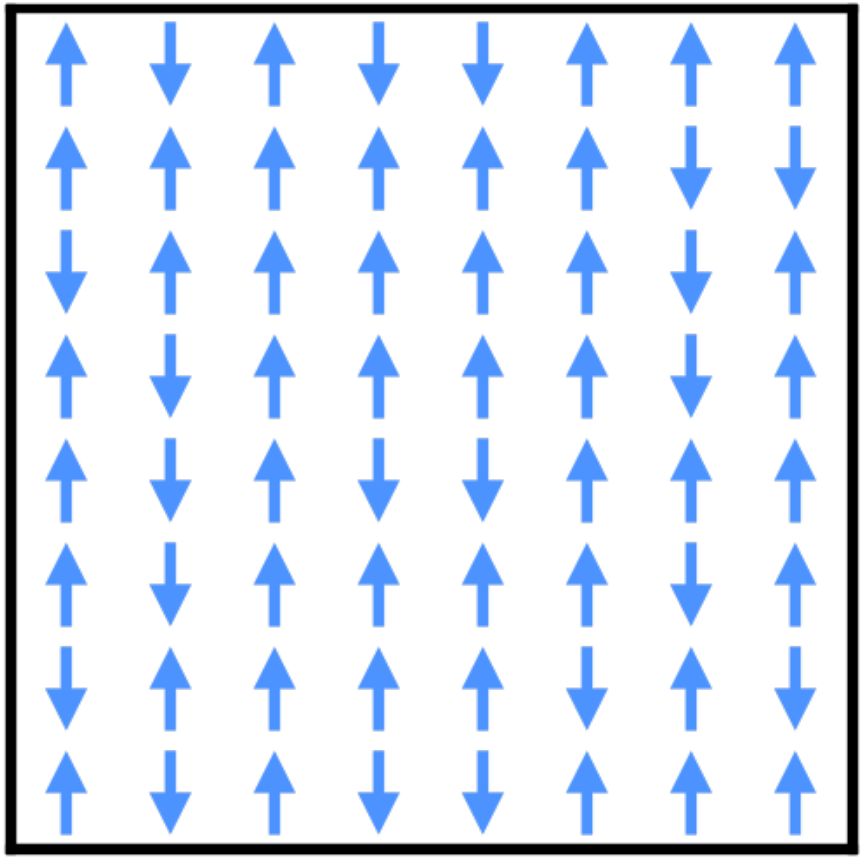
Cluster algorithm, probabilistic (Wolff, 1989)



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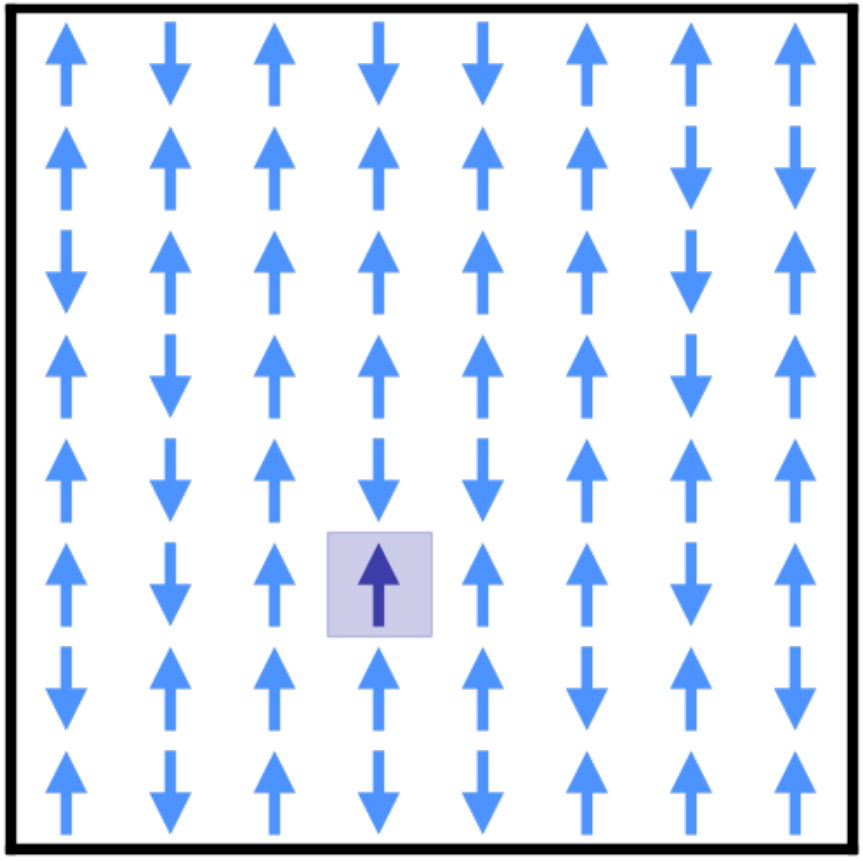

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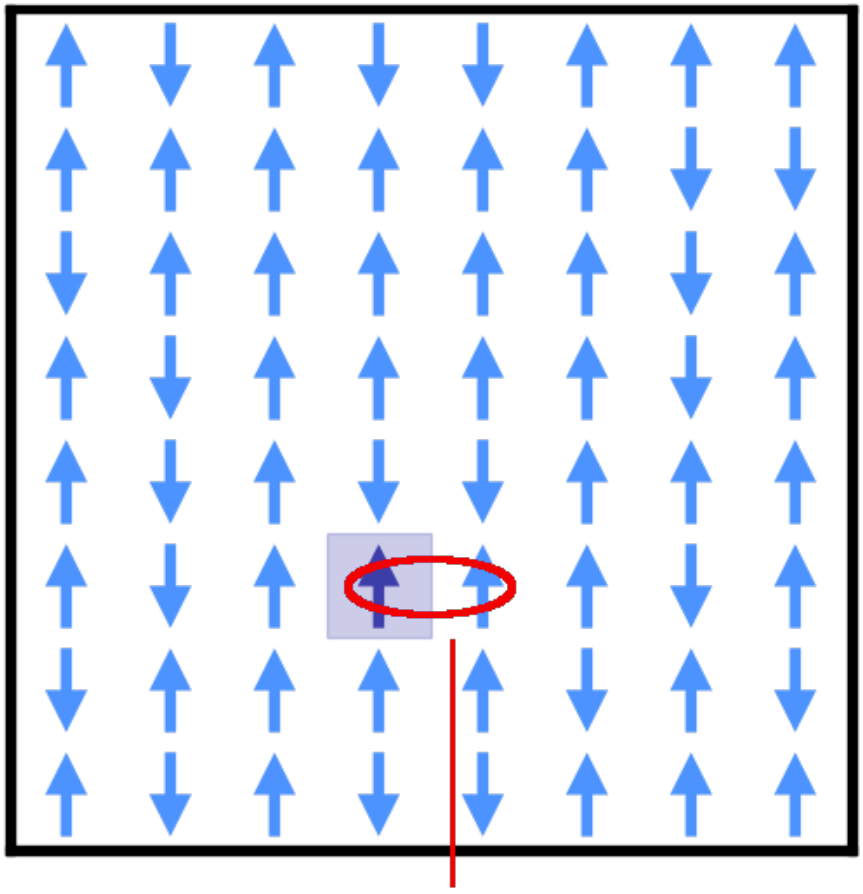

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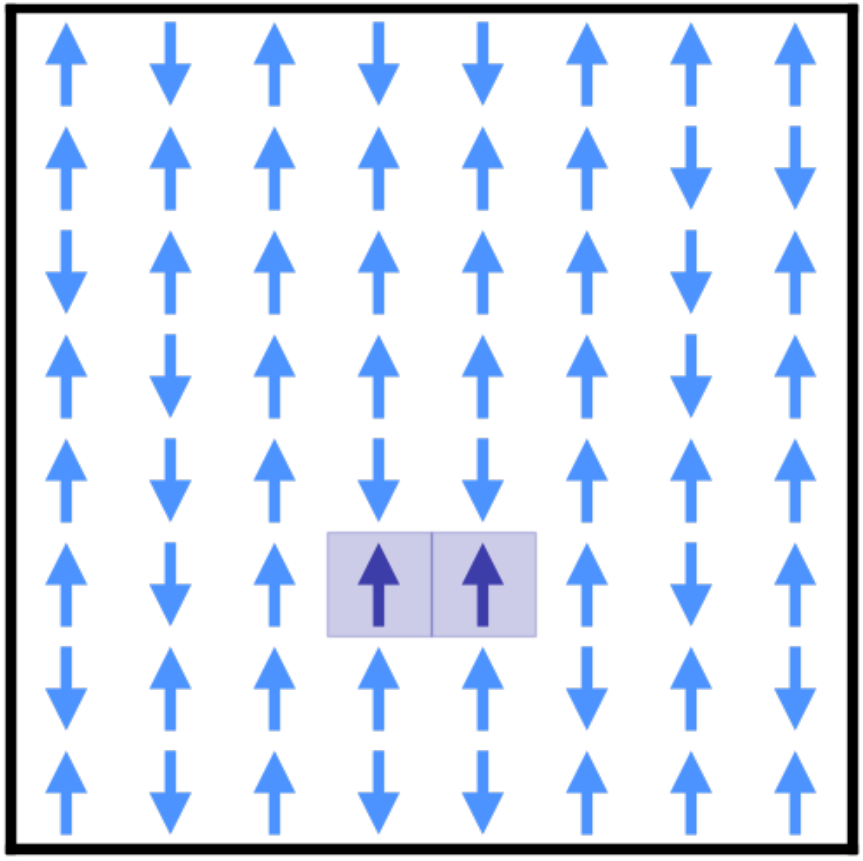

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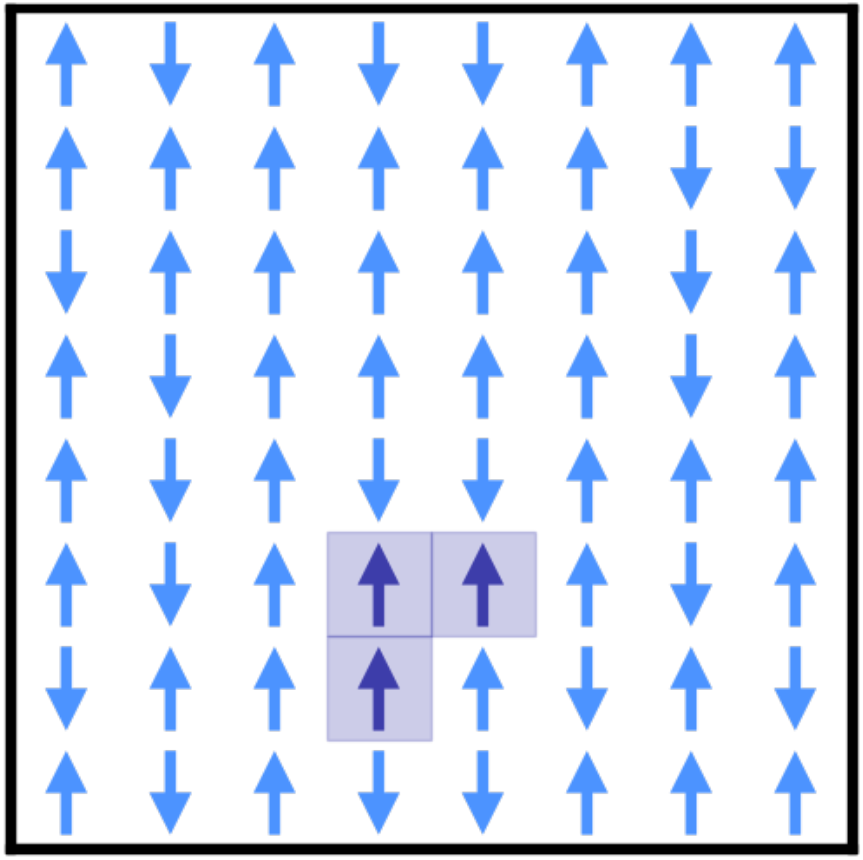

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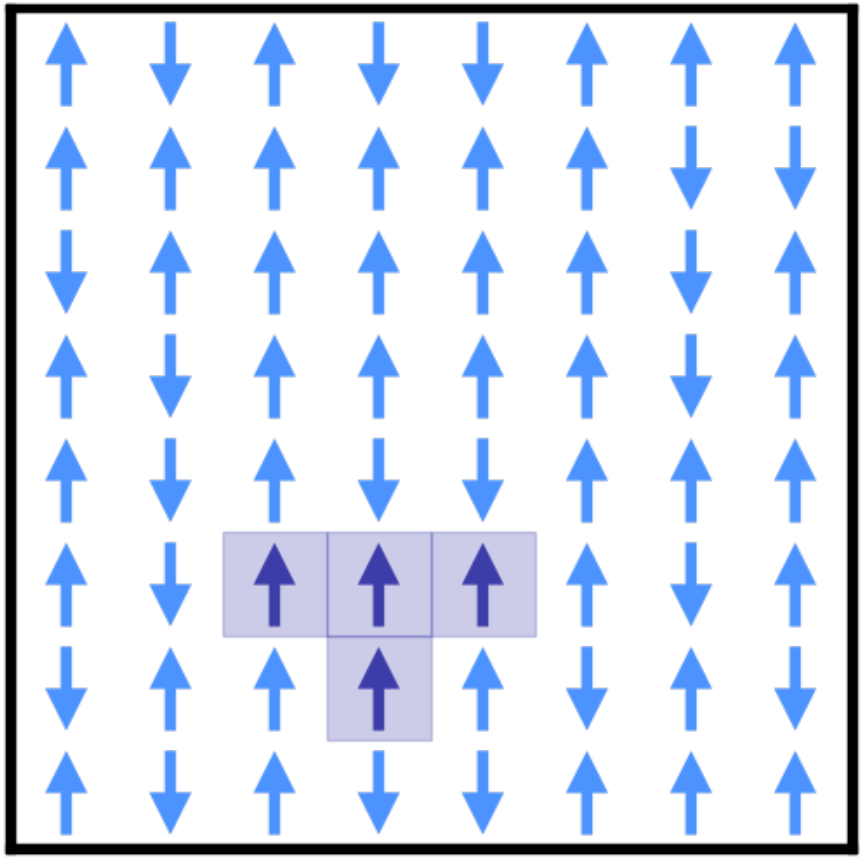

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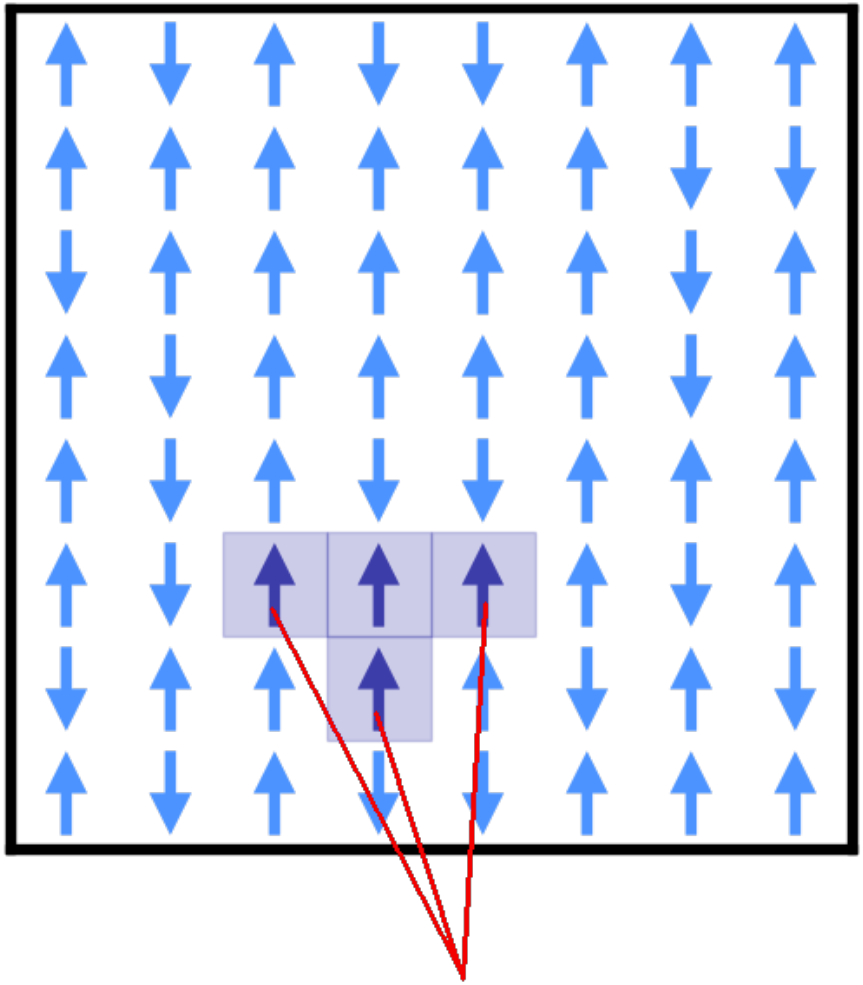
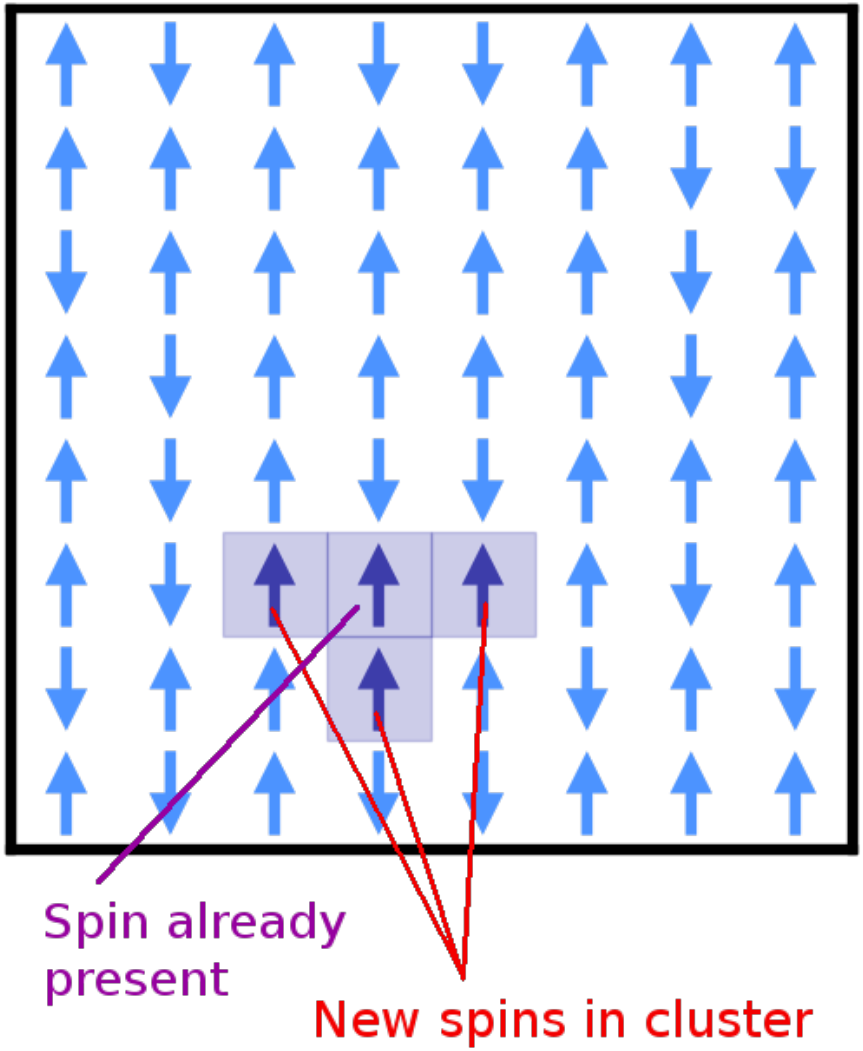


Cluster algorithm, probabilistic (Wolff, 1989)



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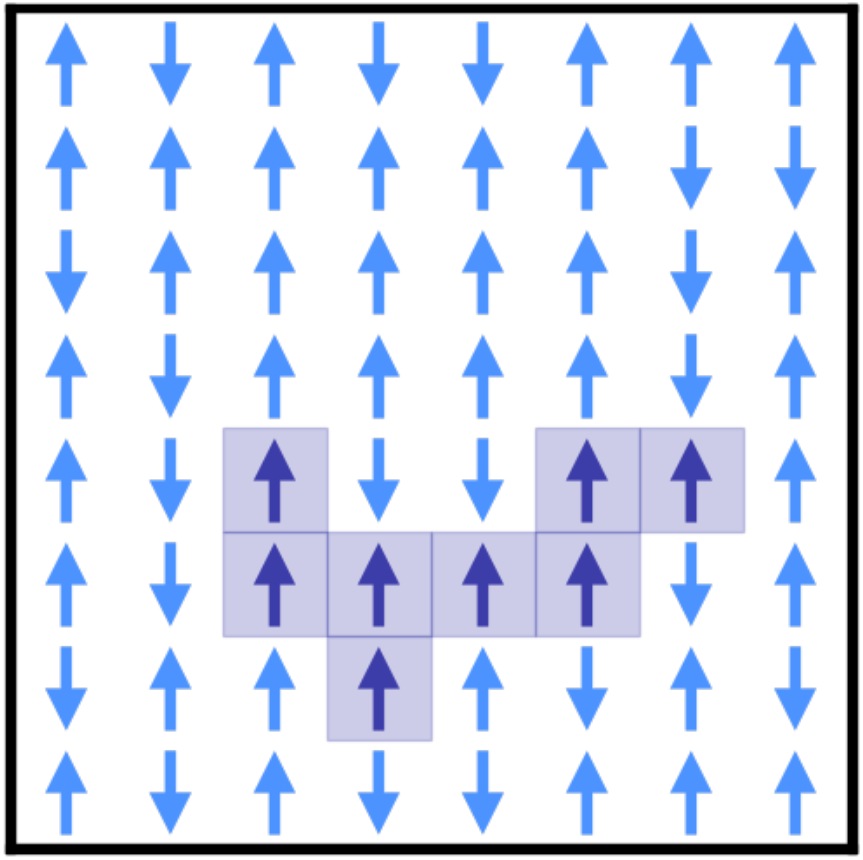

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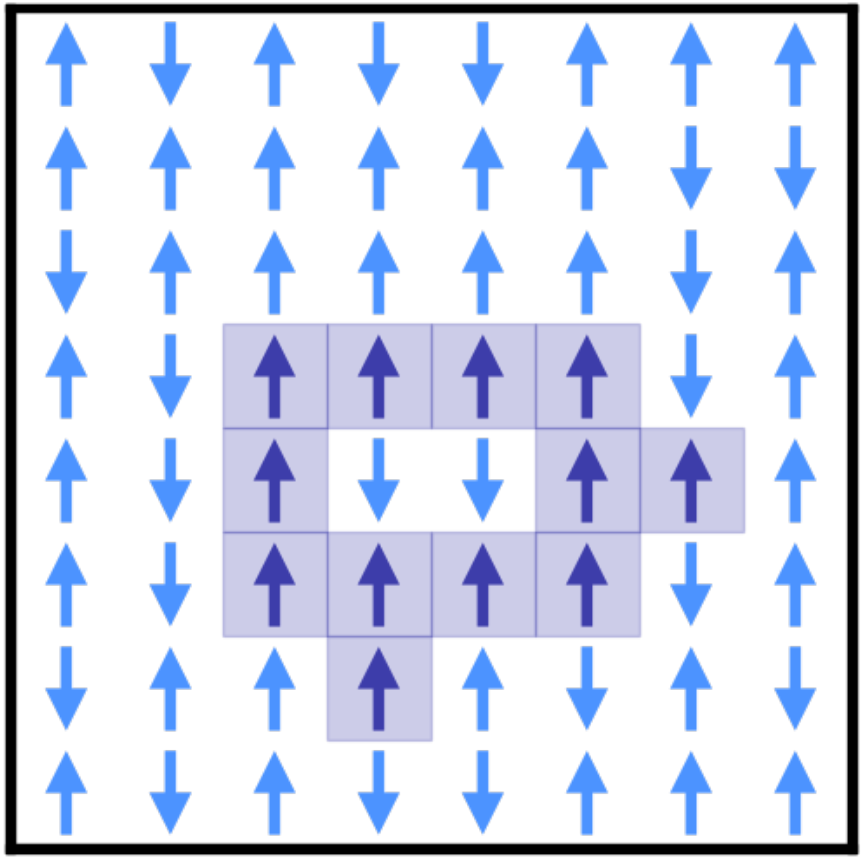

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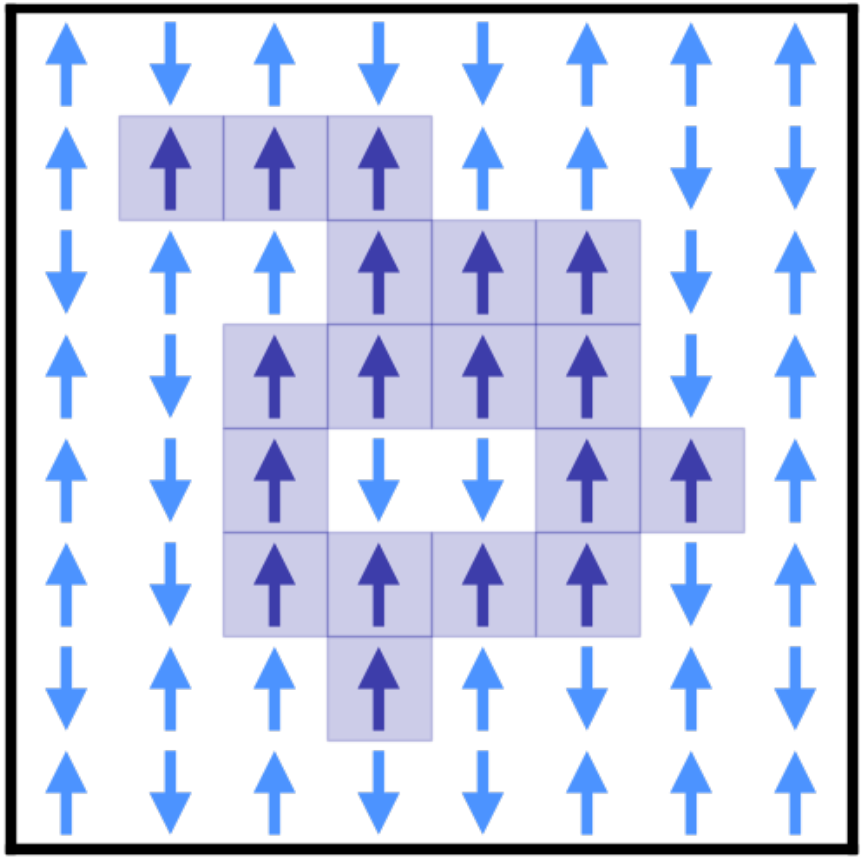
Cluster algorithm, probabilistic (Wolff, 1989)



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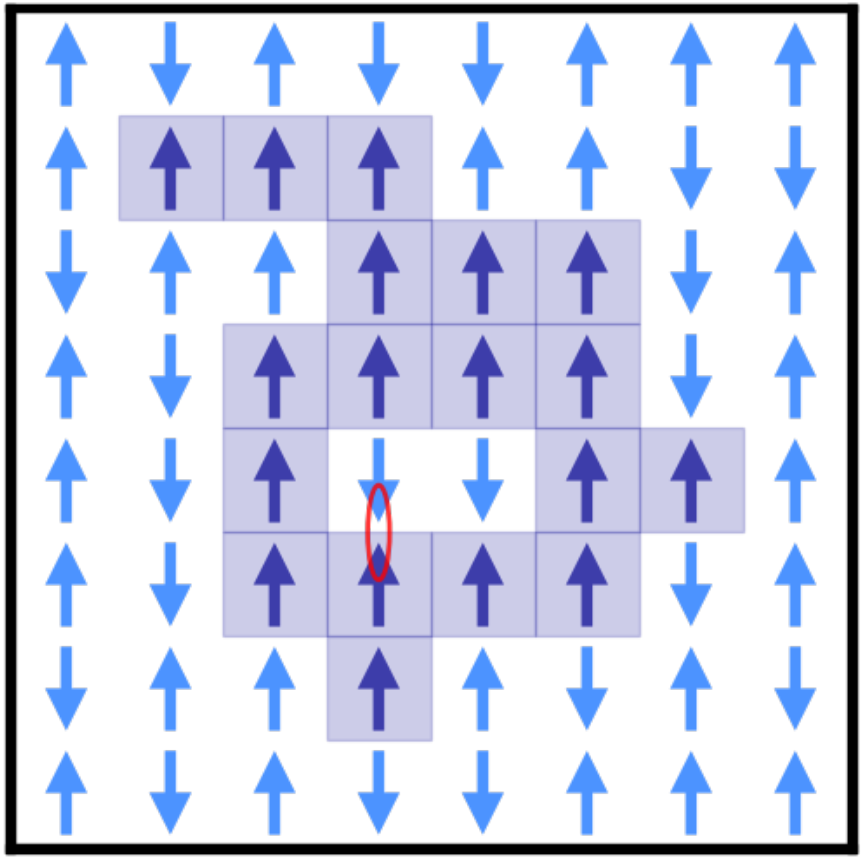

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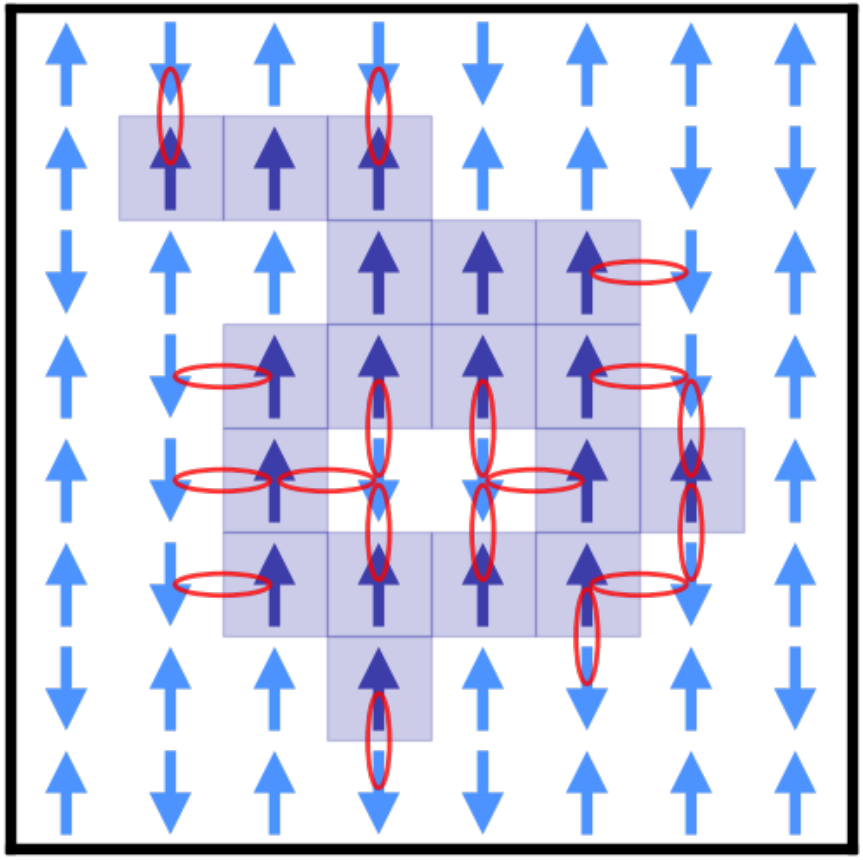

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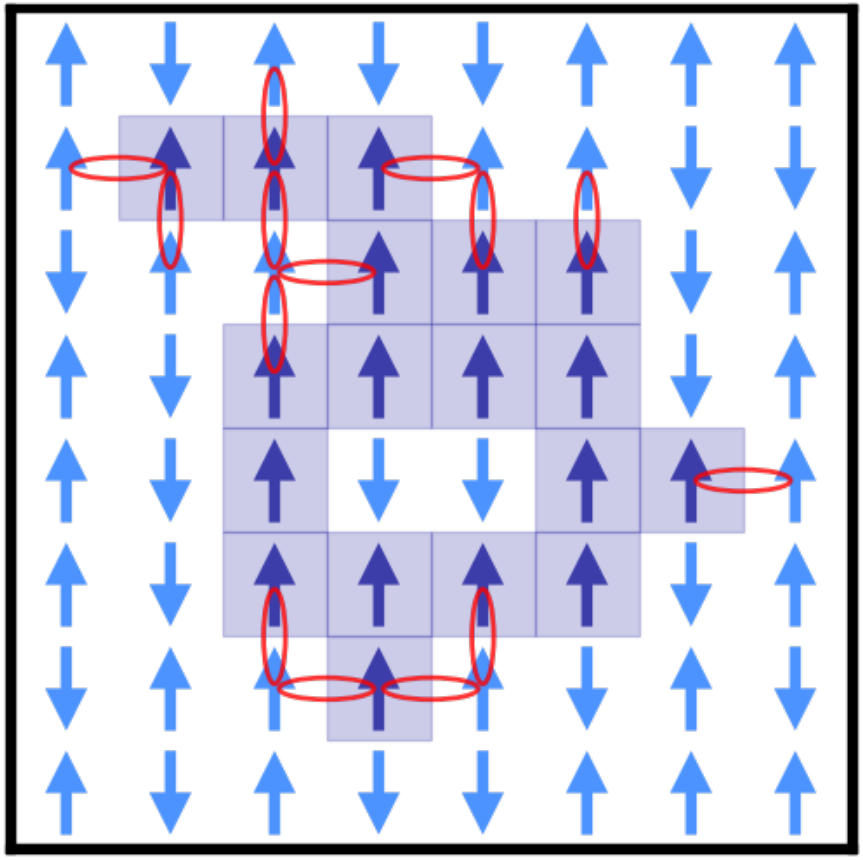

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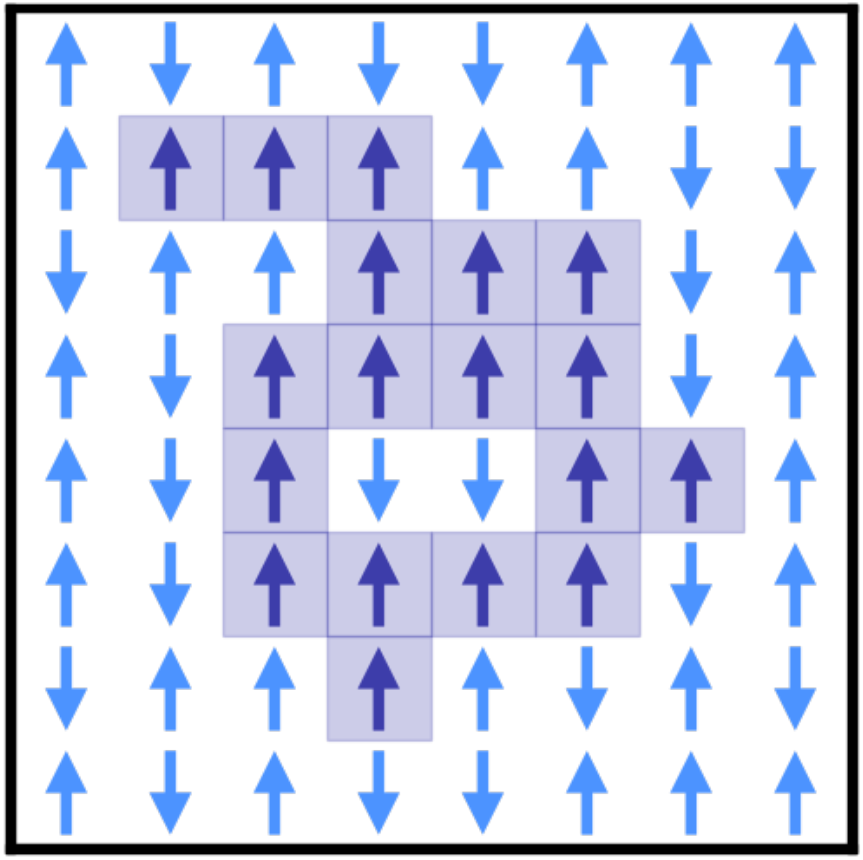

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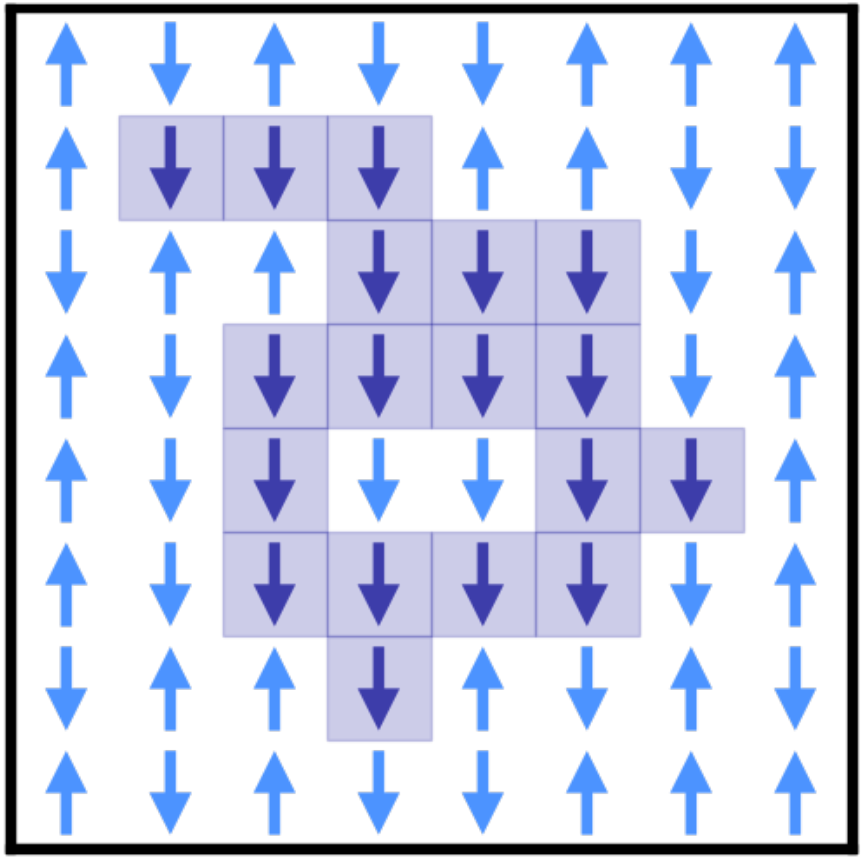

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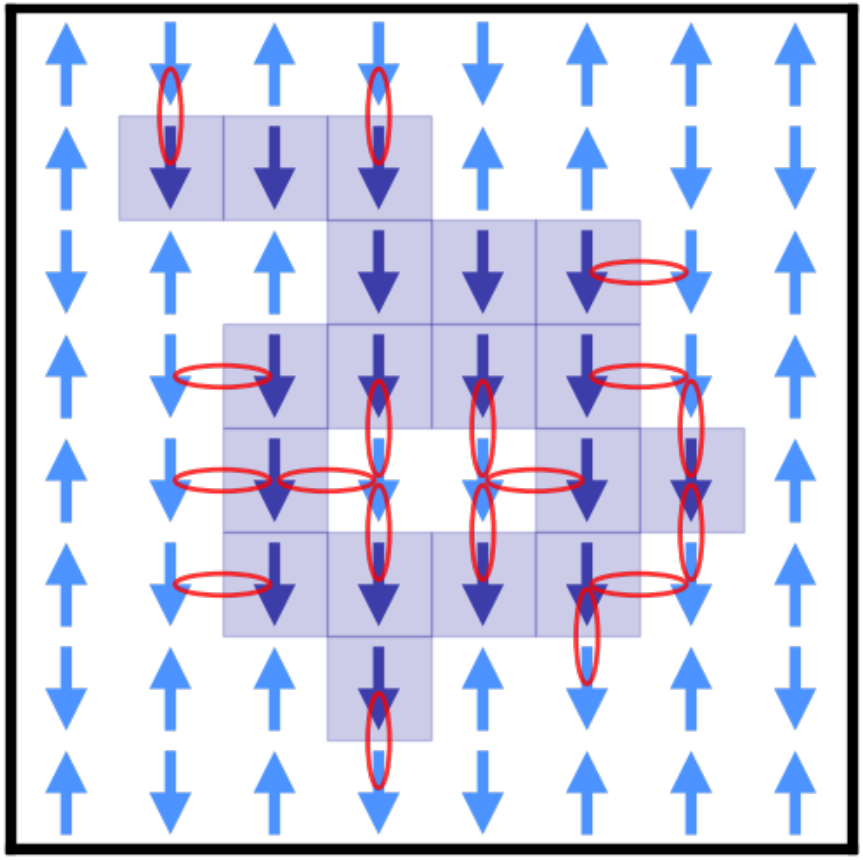
Cluster algorithm, probabilistic (Wolff, 1989)



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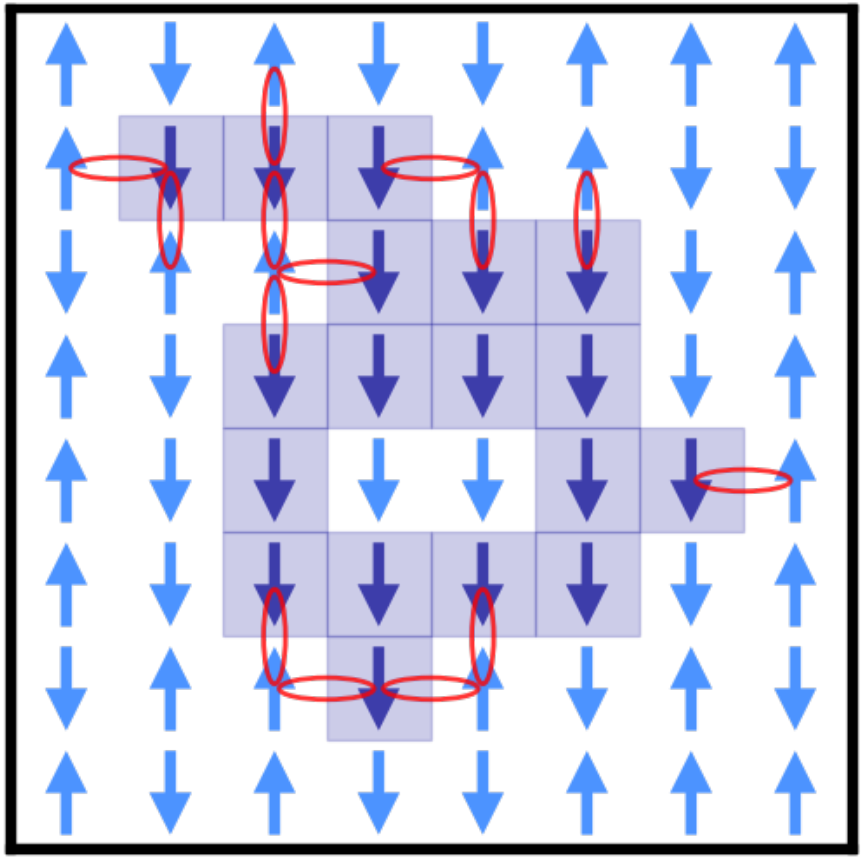
Cluster algorithm, probabilistic (Wolff, 1989)



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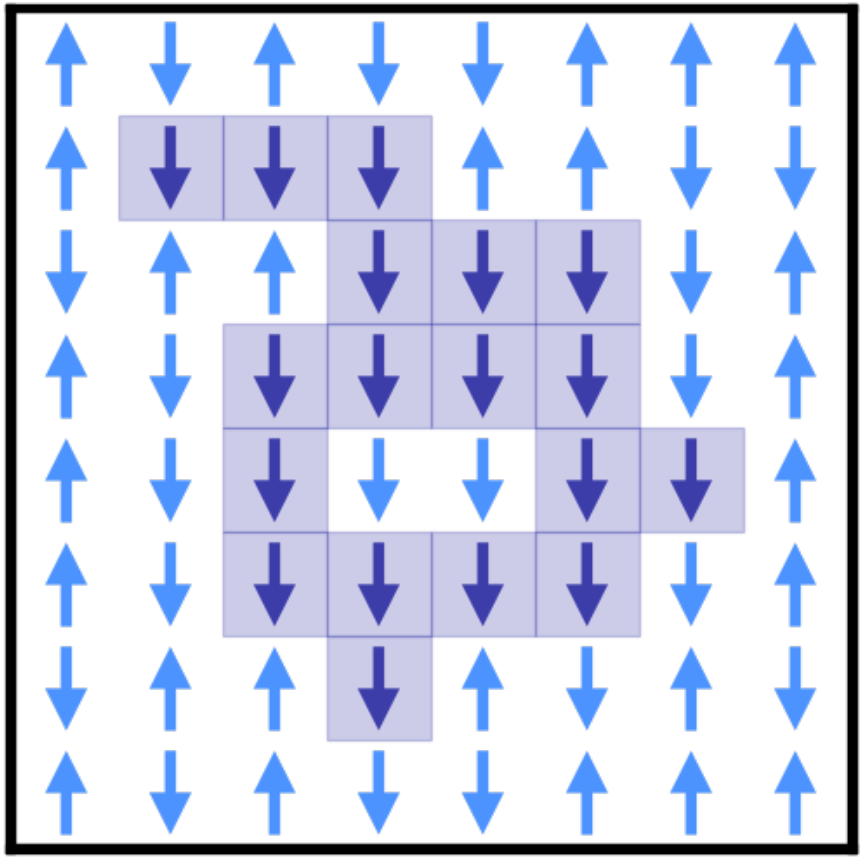
Cluster algorithm, probabilistic (Wolff, 1989)



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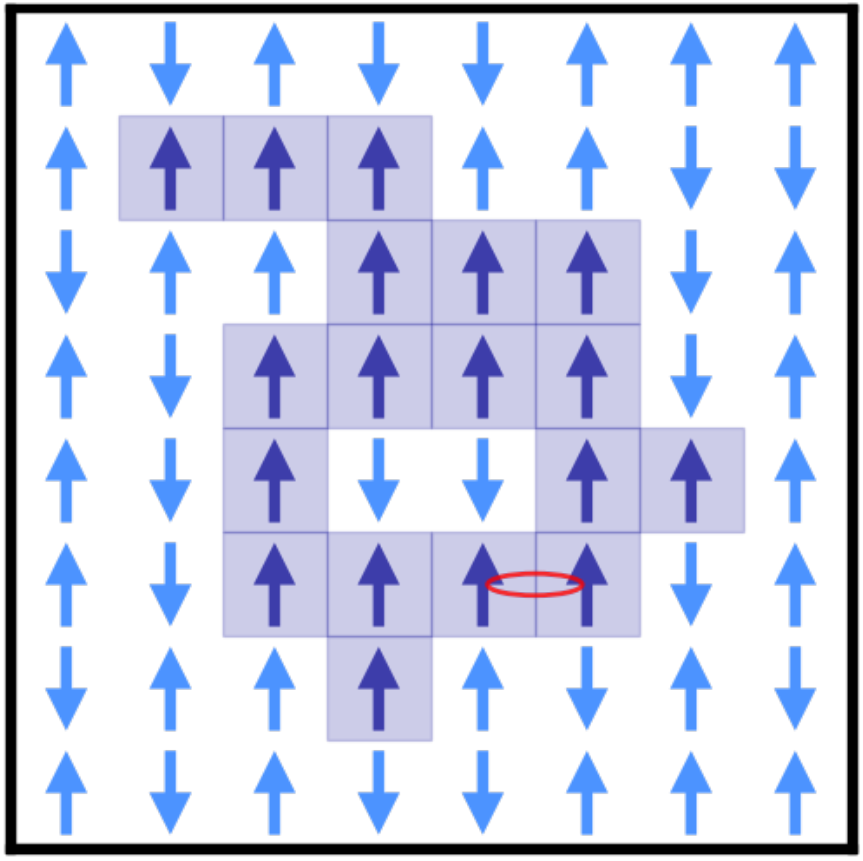
Cluster algorithm, probabilistic (Wolff, 1989)



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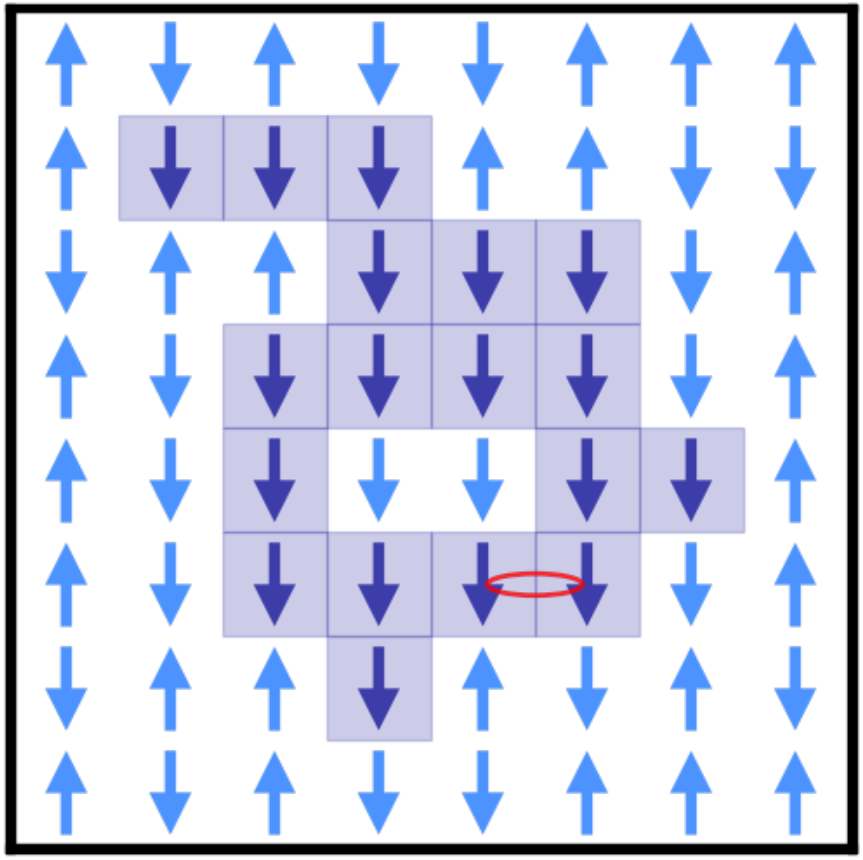
Cluster algorithm, probabilistic (Wolff, 1989)



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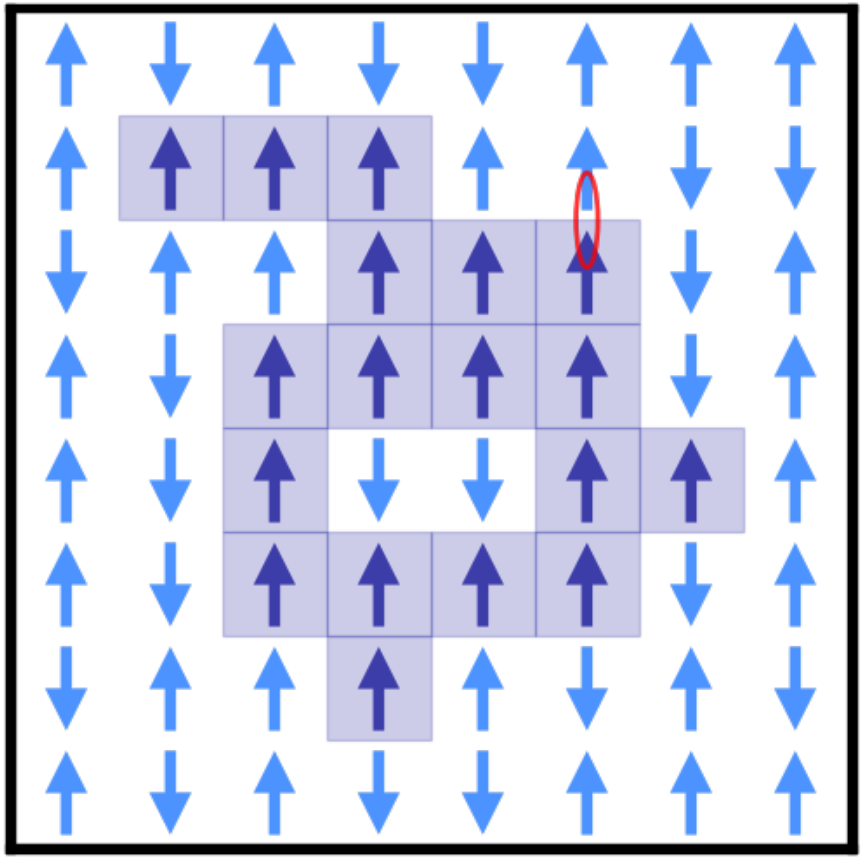
Cluster algorithm, probabilistic (Wolff, 1989)



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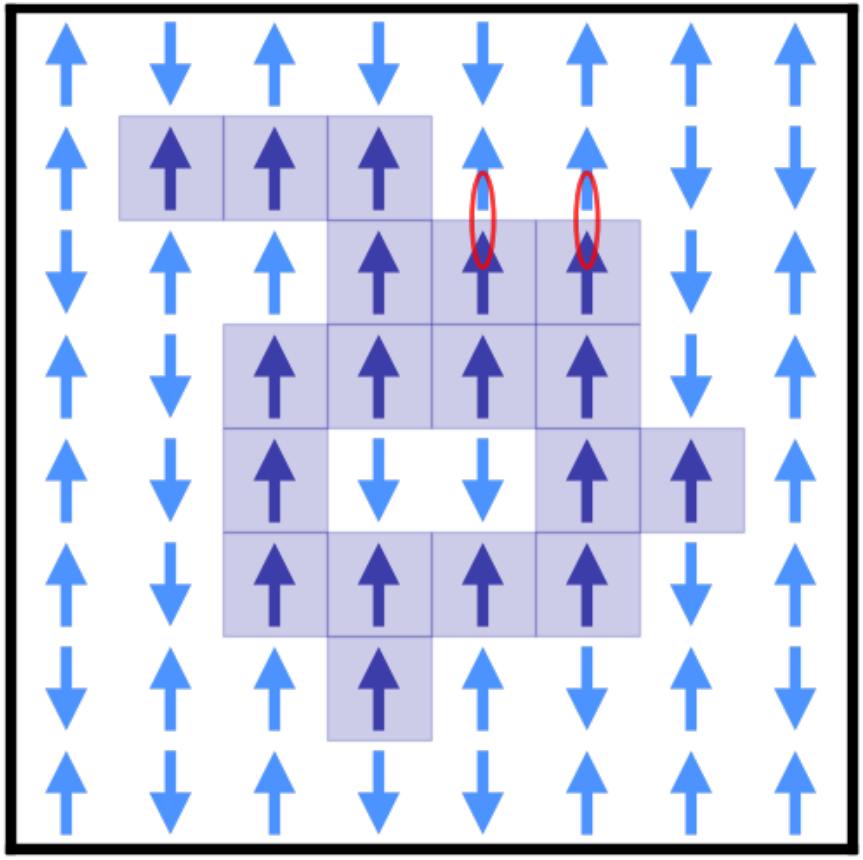
Cluster algorithm, probabilistic (Wolff, 1989)



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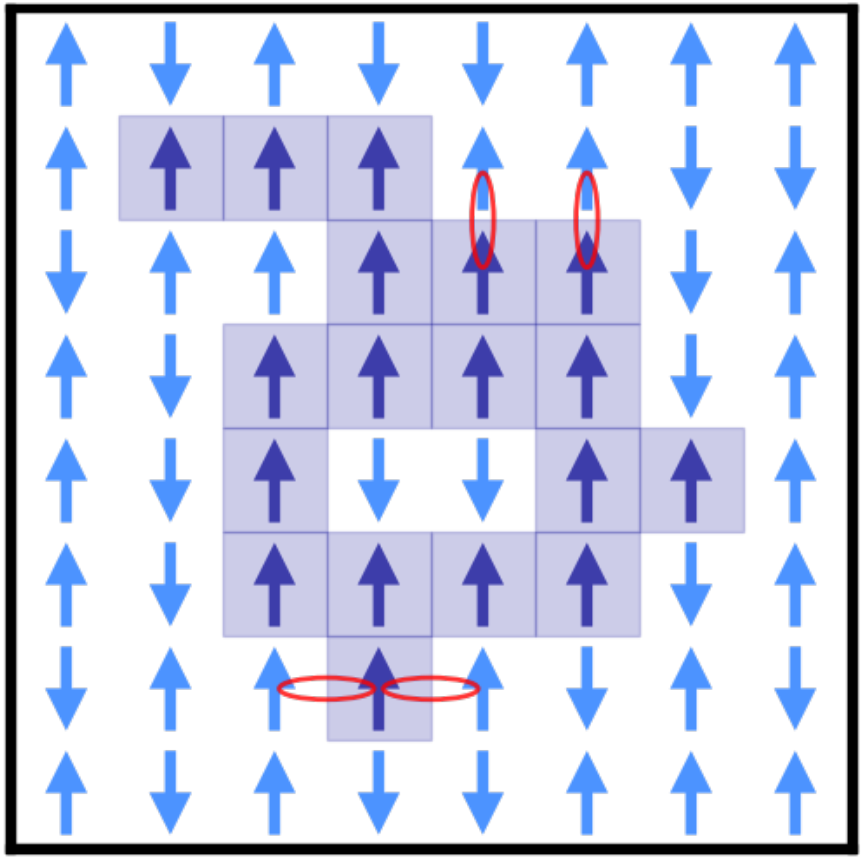
Cluster algorithm, probabilistic (Wolff, 1989)



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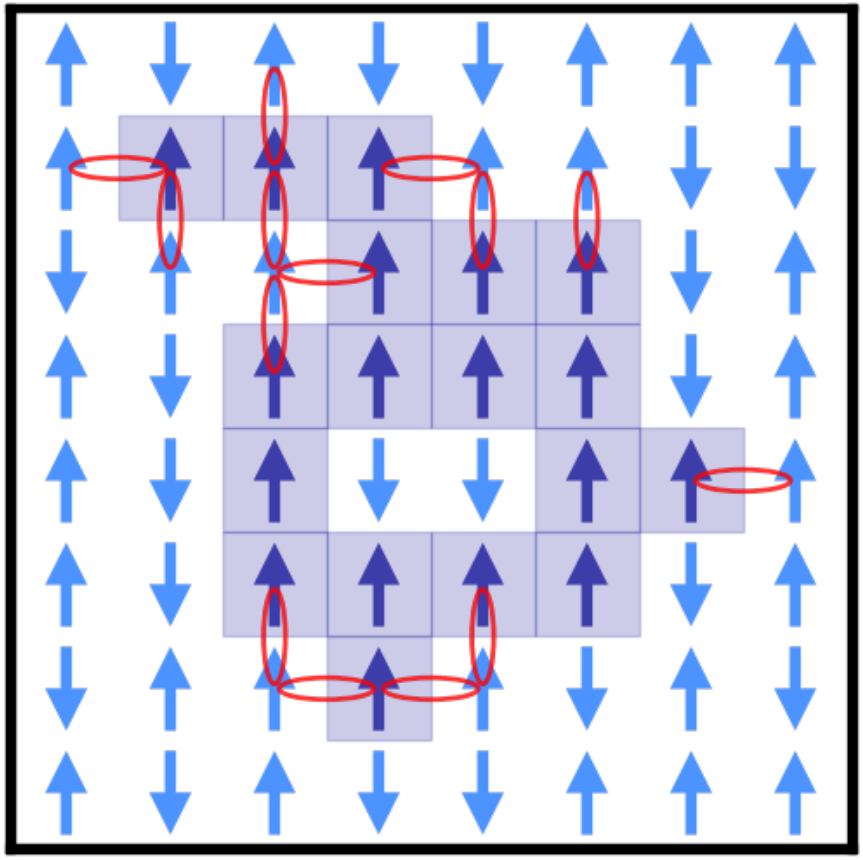
Cluster algorithm, probabilistic (Wolff, 1989)



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Cluster algorithm, probabilistic (Wolff, 1989)

$$\mathcal{A}(a \to b) \propto (1-p)^{14}$$

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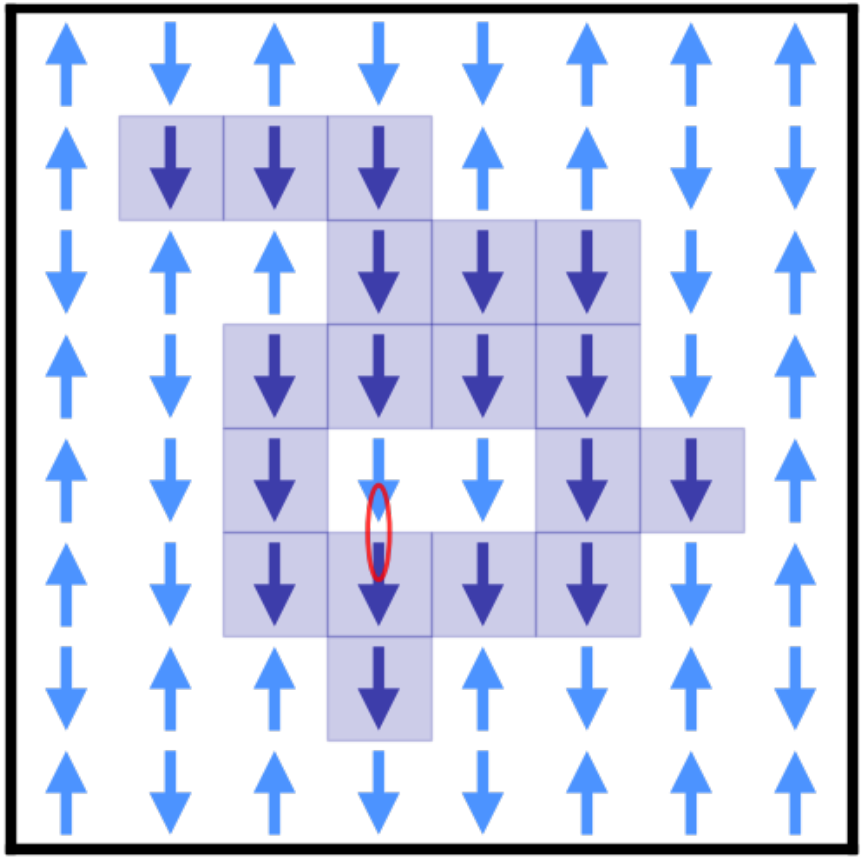
Cluster algorithm, probabilistic (Wolff, 1989)



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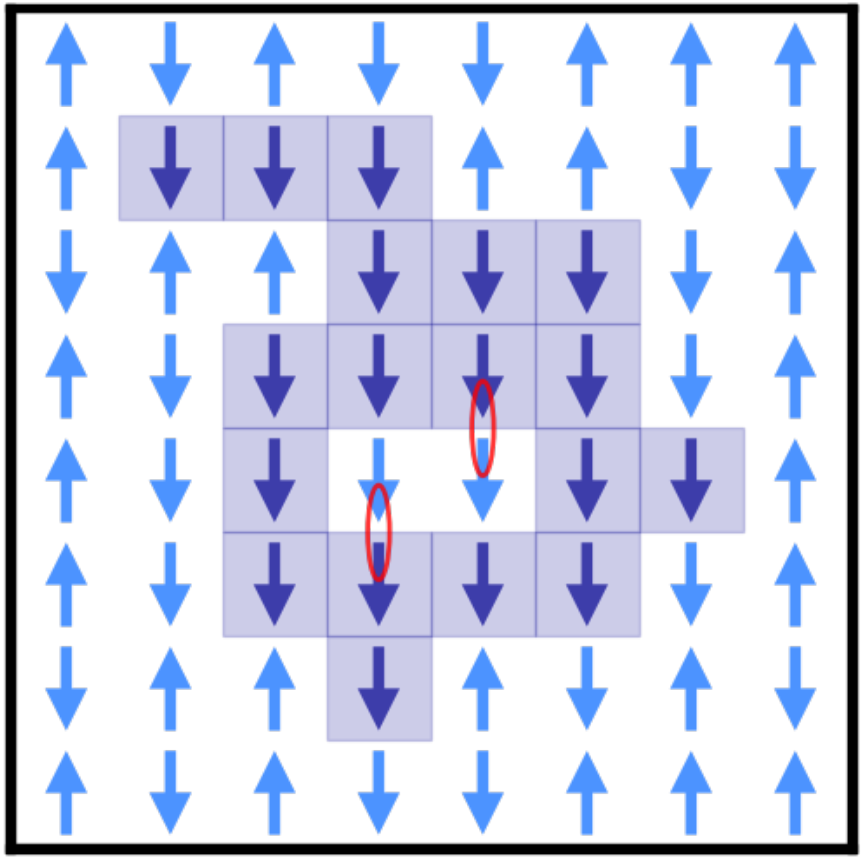
Cluster algorithm, probabilistic (Wolff, 1989)



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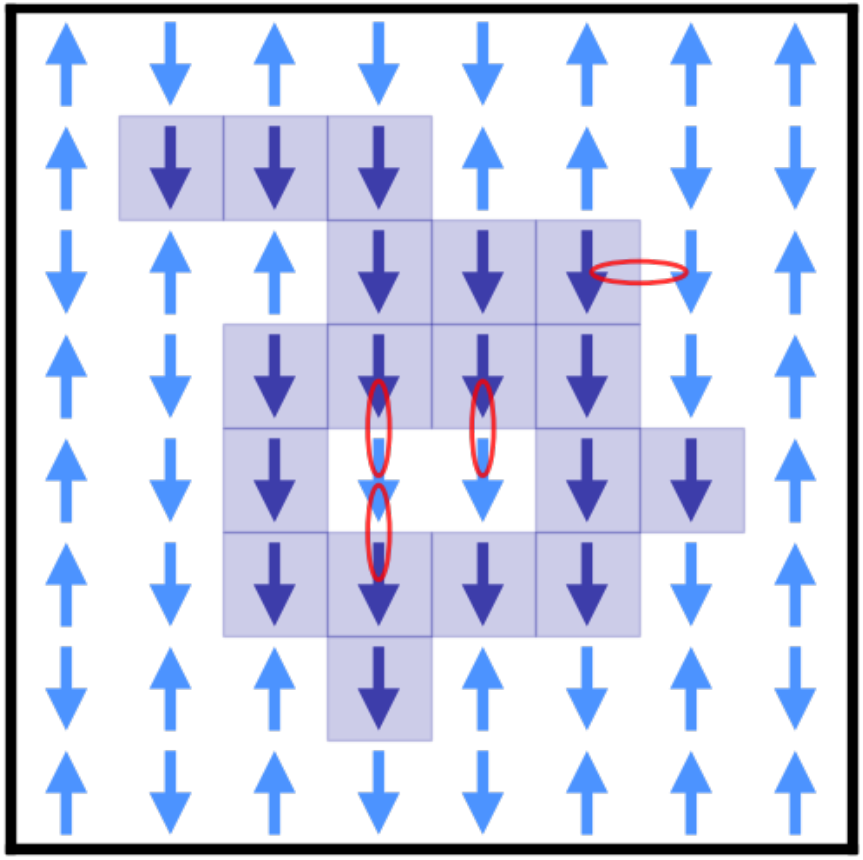

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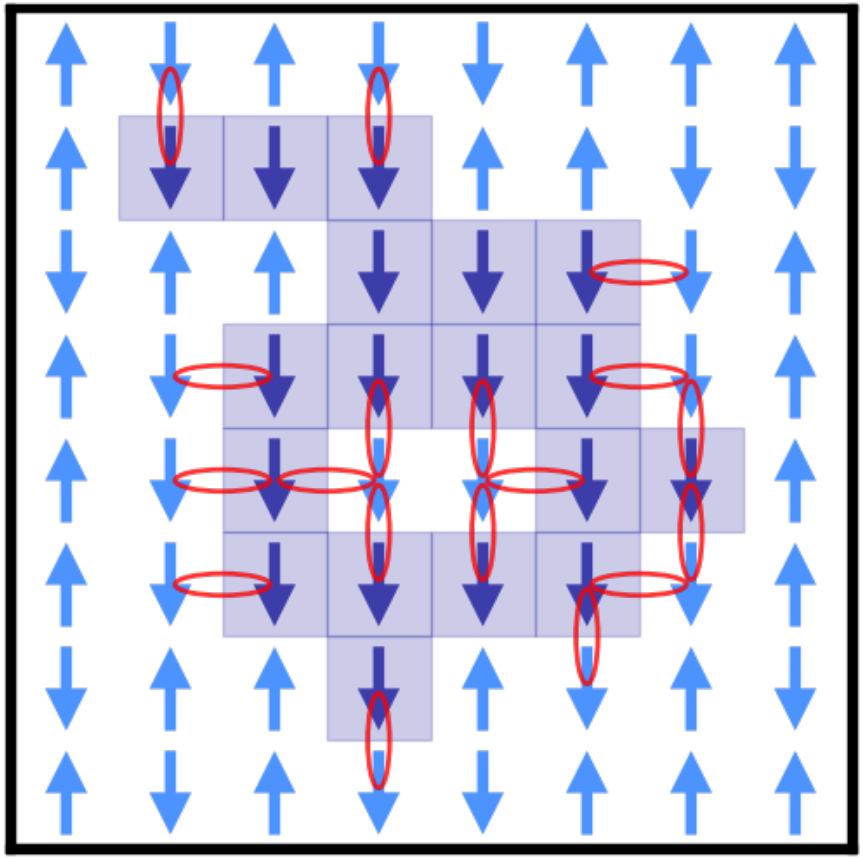
Cluster algorithm, probabilistic (Wolff, 1989)



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Cluster algorithm, probabilistic (Wolff, 1989)

$$\mathcal{A}(b \to a) \propto (1-p)^{18}$$

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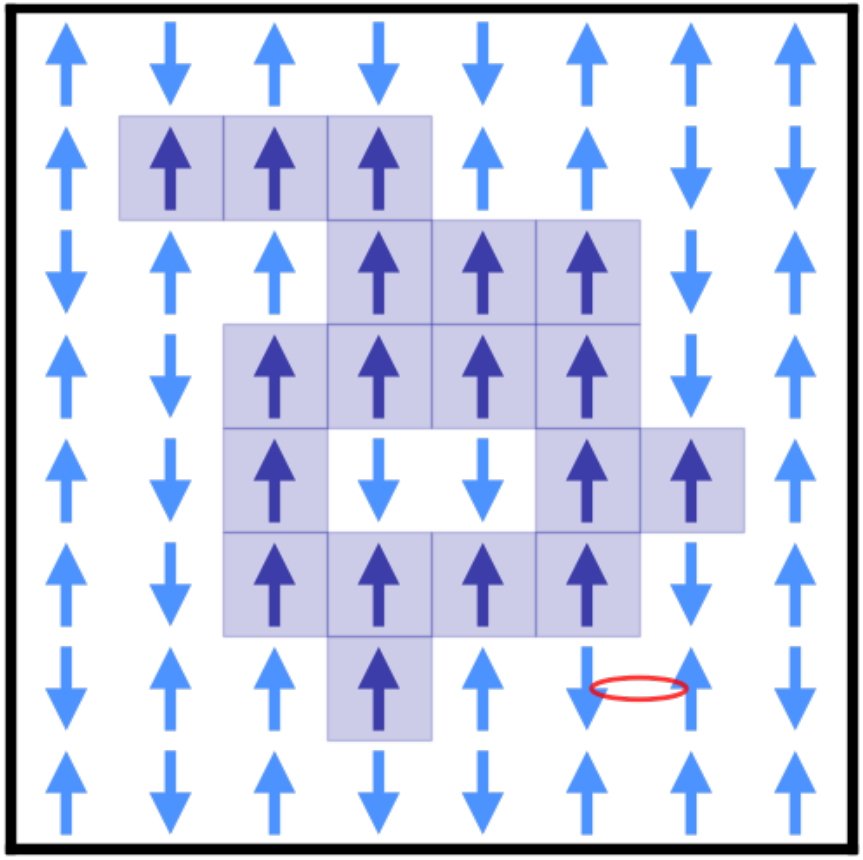
Cluster algorithm, probabilistic (Wolff, 1989)



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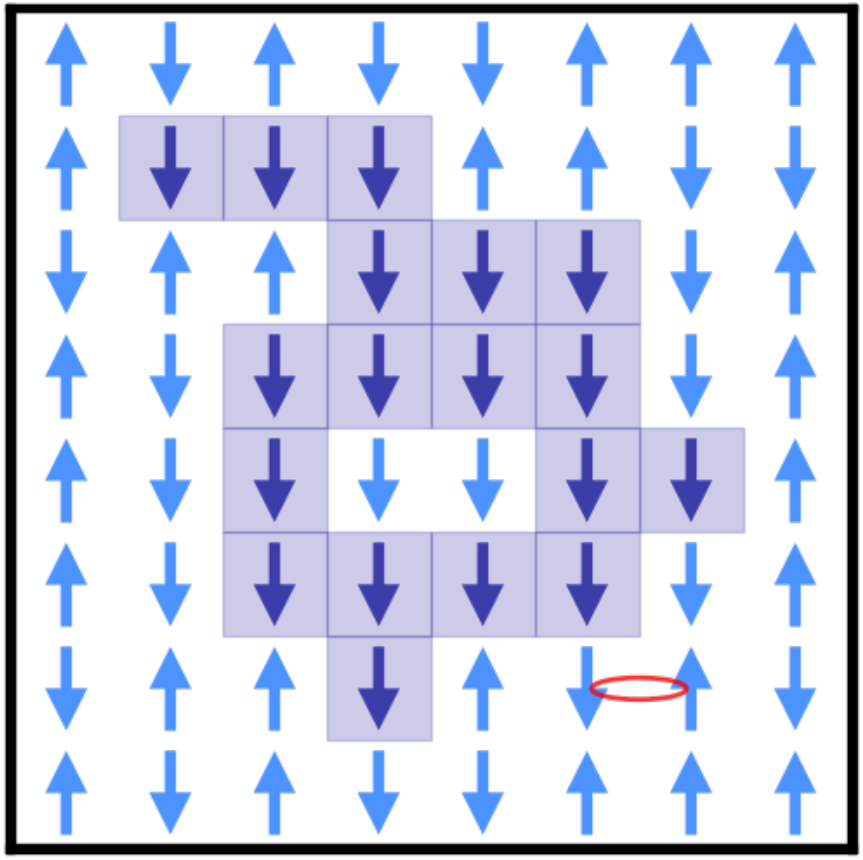
Cluster algorithm, probabilistic (Wolff, 1989)



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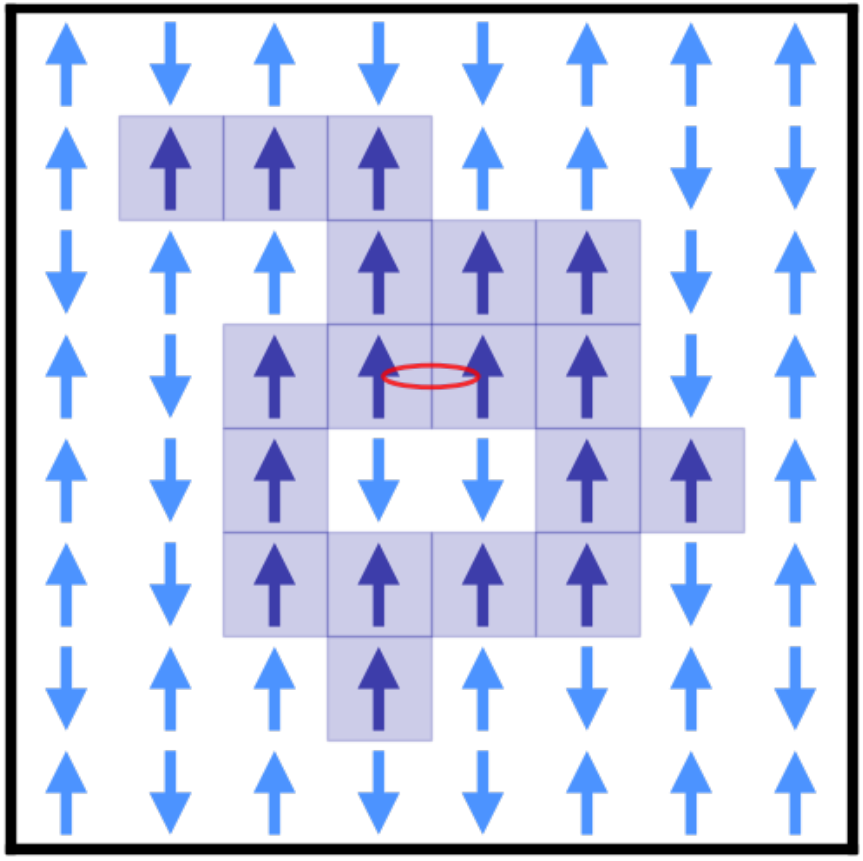
Cluster algorithm, probabilistic (Wolff, 1989)



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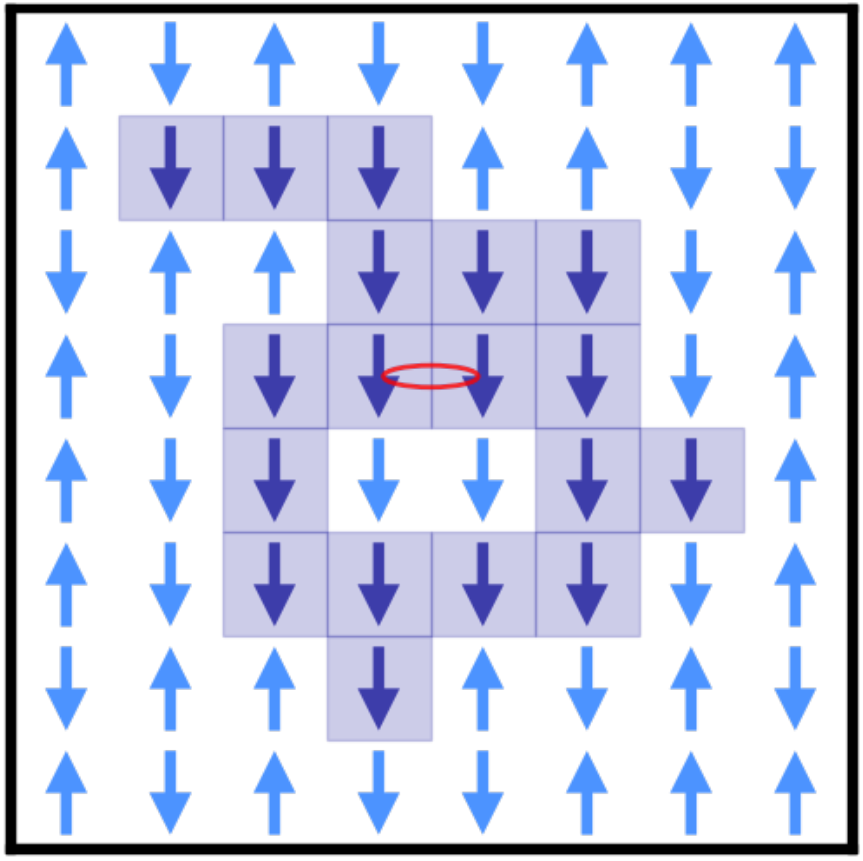
Cluster algorithm, probabilistic (Wolff, 1989)



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Cluster algorithm, probabilistic (Wolff, 1989)

$$\text{energy of the boundary}$$

$$=$$

$$n_1 - n_2$$

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Cluster algorithm, probabilistic (Wolff, 1989)

$$\text{energy of the boundary}$$

$$=$$

$$n_2 - n_1$$

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Cluster algorithm, probabilistic (Wolff, 1989)

$$n_1 = 18, \quad n_2 = 14$$

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Detailed balance (Metropolis-Hastings)

$$e^{-\beta(n_1-n_2)}(1-p)^{n_2}p^{\mathrm{acc}}(a\to b) = e^{-\beta(n_2-n_1)}(1-p)^{n_1}p^{\mathrm{acc}}(b\to a)$$

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Detailed balance (Metropolis-Hastings)

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$\pi(a)$ (depends on energy across boundaries)

Département de Physique
École normale supérieure

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$\mathcal{A}(a\to b)$ (probability to stop construction)

$\pi(a)$ (depends on energy across boundaries)

Département de Physique
École normale supérieure

Detailed balance (Metropolis-Hastings)

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- $\mathcal{A}(a\to b)$ (probability to stop construction)
- $\pi(a)$ (depends on energy across boundaries)

$$p^{\mathrm{acc}}(a\to b) = \min\left[1, \frac{e^{-\beta(n_2-n_1)}(1-p)^{n_1}}{e^{-\beta(n_1-n_2)}(1-p)^{n_2}}\right]$$

Département de Physique
École normale supérieure

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$$= \min\left[1, \left(\frac{e^{-2\beta}}{1-p}\right)^{n_2}\left(\frac{1-p}{e^{-2\beta}}\right)^{n_1}\right]$$

Département de Physique
École normale supérieure

Detailed balance (Metropolis-Hastings)

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$$= \min\left[1, \left(\frac{e^{-2\beta}}{1-p}\right)^{n_2}\left(\frac{1-p}{e^{-2\beta}}\right)^{n_1}\right]$$

$1-p = e^{-2\beta}$ magic value

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$$e^{-\beta(n_1-n_2)}(1-p)^{n_2}p^{\mathrm{acc}}(a\to b) = e^{-\beta(n_2-n_1)}(1-p)^{n_1}p^{\mathrm{acc}}(b\to a)$$

- $\mathcal{A}(a\to b)$ (probability to stop construction)
- $\pi(a)$ (depends on energy across boundaries)

$$p^{\mathrm{acc}}(a\to b) = \min\left[1, \frac{e^{-\beta(n_2-n_1)}(1-p)^{n_1}}{e^{-\beta(n_1-n_2)}(1-p)^{n_2}}\right]$$

$$= 1$$

$$1-p = e^{-2\beta} \qquad \text{magic value}$$

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cluster-ising.py

```
import random, math

L = 100
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N)
                                        for i in range(N)}
T = 2.5
p  = 1.0 - math.exp(-2.0 / T)
nsteps = 10000
S = [random.choice([1, -1]) for k in range(N)]
for step in range(nsteps):
    k = random.randint(0, N - 1)
    Pocket, Cluster = [k], [k]
    while Pocket != []:
        j = random.choice(Pocket)
        for l in nbr[j]:
            if S[l] == S[j] and l not in Cluster \
                    and random.uniform(0.0, 1.0) < p:
                Pocket.append(l)
                Cluster.append(l)
        Pocket.remove(j)
    for j in Cluster:
        S[j] *= -1
```

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Running cluster-ising.py

Metropolis algorithm (reminder)

$$\pi(a)\,\mathcal{A}(a \to b)\,p^{\mathrm{acc}}(a \to b) = \pi(b)\,\mathcal{A}(b \to a)\,p^{\mathrm{acc}}(b \to a)$$

$$\mathcal{A}(a \to b) = \mathcal{A}(b \to a)$$

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Metropolis algorithm (reminder)

$$\pi(a)\,\mathcal{A}(a \to b)\,p^{\mathrm{acc}}(a \to b) = \pi(b)\,\mathcal{A}(b \to a)\,p^{\mathrm{acc}}(b \to a)$$

$$\mathcal{A}(a \to b) = \mathcal{A}(b \to a)$$

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Heatbath algorithm

$$\pi(a)\,\mathcal{A}(a \to b)\,p^{\mathrm{acc}}(a \to b) = \pi(b)\,\mathcal{A}(b \to a)\,p^{\mathrm{acc}}(b \to a)$$

$$\mathcal{A}(a \to b) \propto \pi(b); \quad \mathcal{A}(b \to a) \propto \pi(a)$$

- Acceptance probabilities $= 1$
- Apply to subsystem

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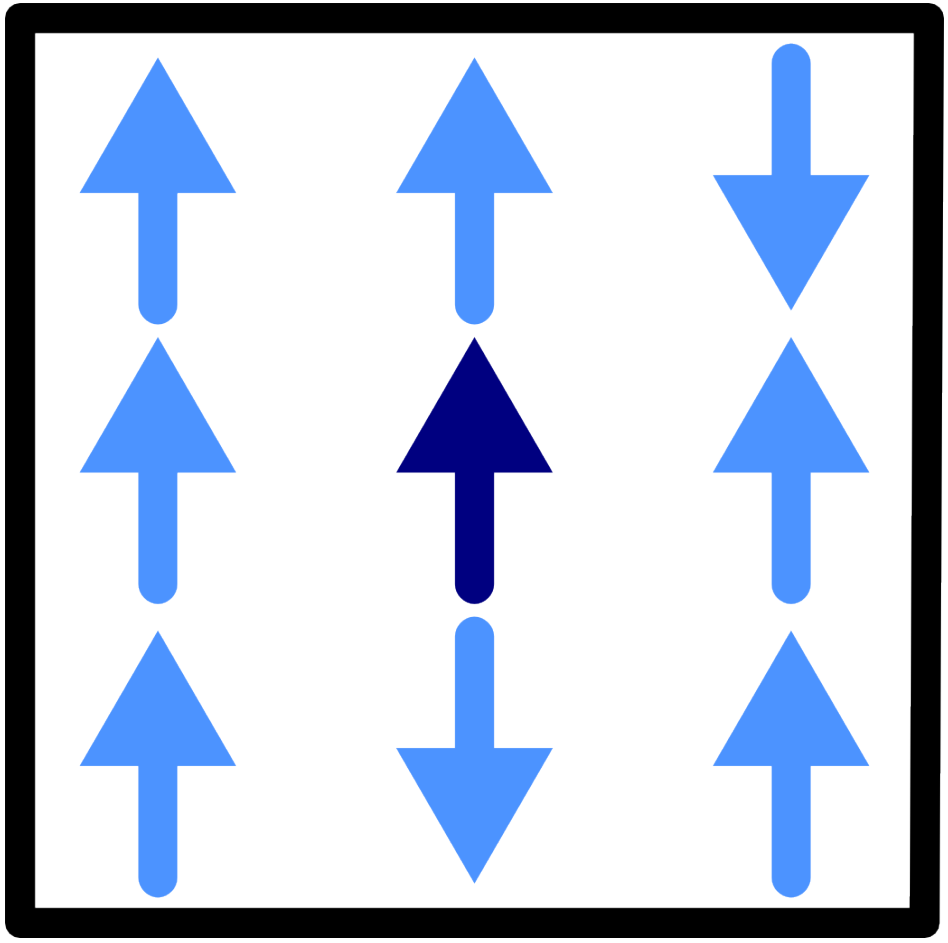
Heatbath algorithm



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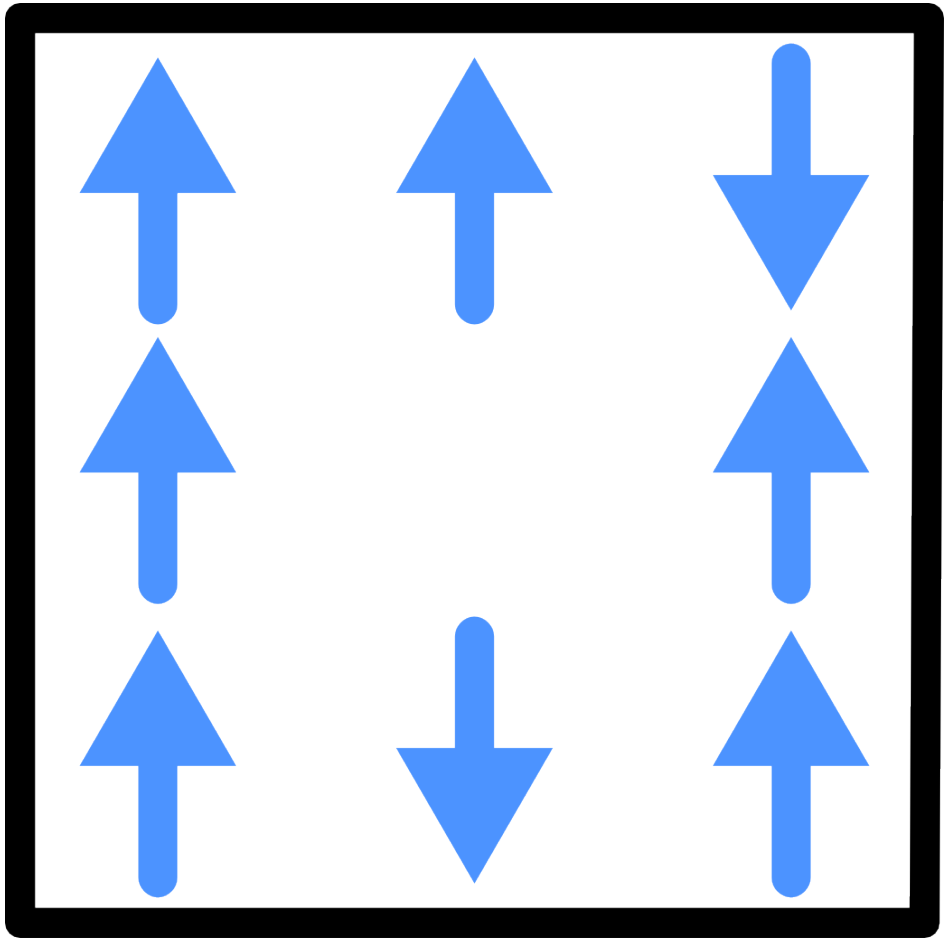
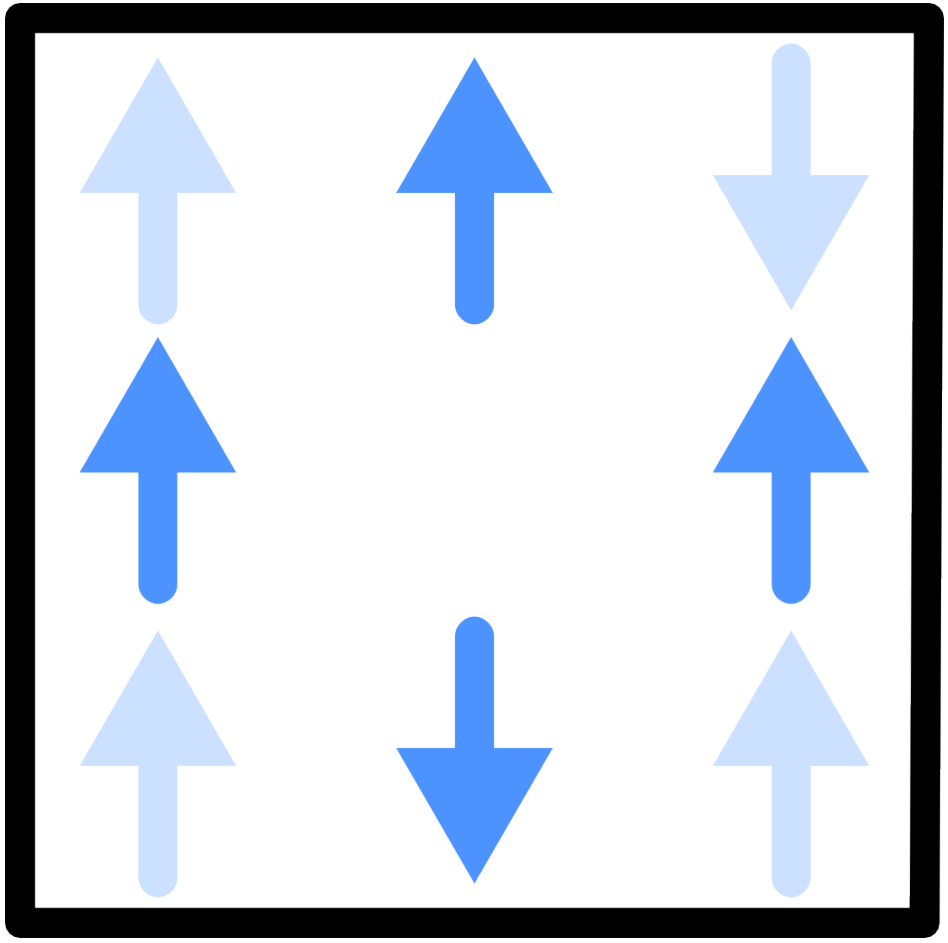
Heatbath algorithm



Heatbath algorithm



Heatbath algorithm

$$\pi^+ = \frac{\mathrm{e}^{\beta h}}{\mathrm{e}^{-\beta h} + \mathrm{e}^{\beta h}}$$

$$\pi^- = \frac{\mathrm{e}^{-\beta h}}{\mathrm{e}^{-\beta h} + \mathrm{e}^{\beta h}}$$

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heatbath-ising.py

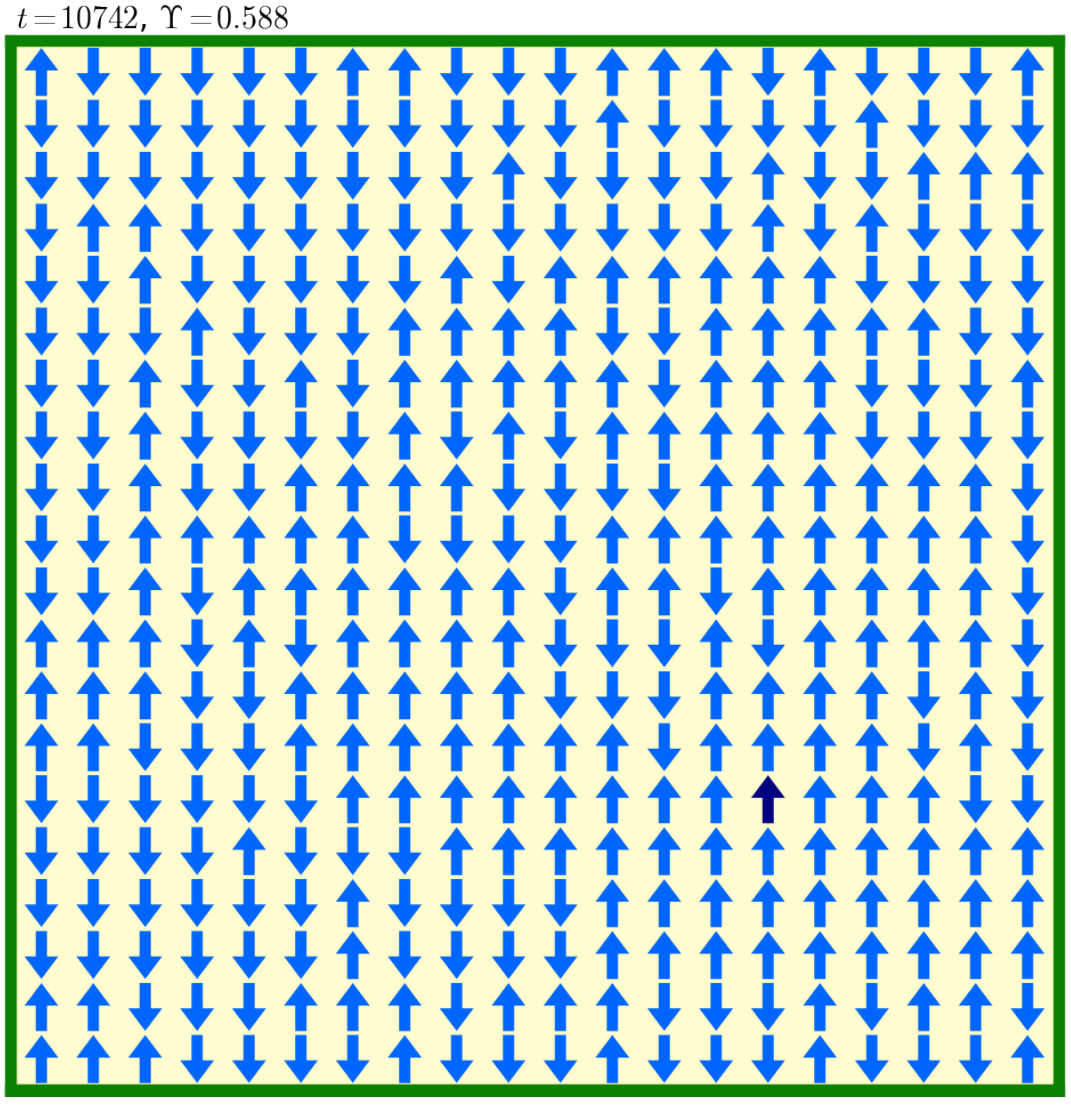
```
import random, math

L = 16
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N) \
                                        for i in range(N)}
nsteps = 100000
beta = 0.5
S = [random.choice([1, -1]) for i in range(N)]
random.seed('123456')
for step in range(nsteps):
    k = random.randrange(N)
    Upsilon = random.uniform(0.0, 1.0)
    h = sum(S[nn] for nn in nbr[k])
    S[k] = -1
    if Upsilon < 1.0 / (1.0 + math.exp(-2.0 * beta * h)):
        S[k] = 1
```

Running heatbath-ising.py from all up

Running heatbath-ising.py from all down

final configuration "up"



- Propp & Wilson 1996

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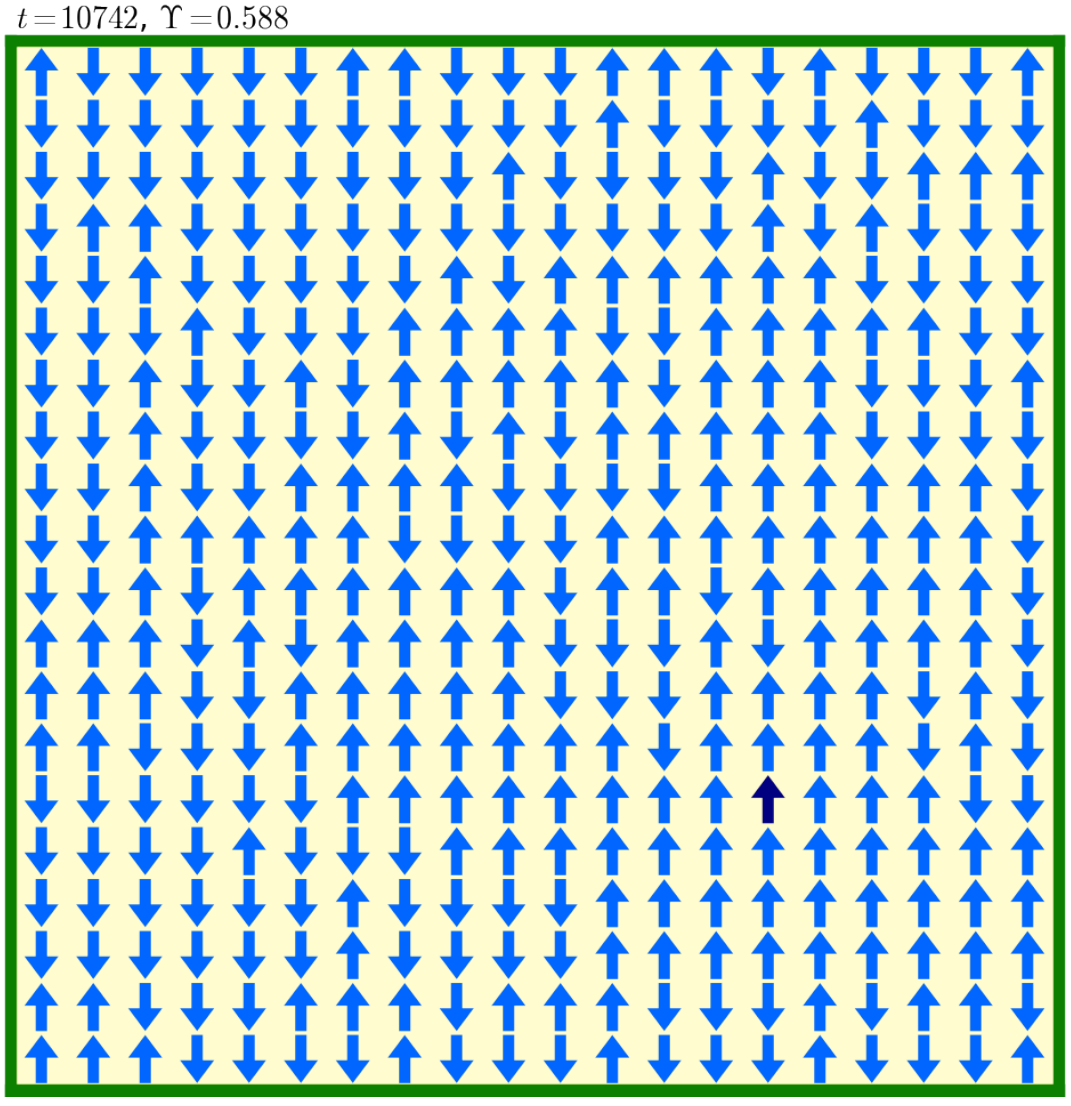
final configuration "down"



- Propp & Wilson 1996

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Coupling in heatbath-ising.py

```
import random, math

L = 16
N = L * L
nbr = {i : ((i // L) * L + (i + 1) % L, (i + L) % N,
            (i // L) * L + (i - 1) % L, (i - L) % N) \
                                        for i in range(N)}
nsteps = 100000
beta = 0.5
S = [random.choice([1, -1]) for i in range(N)]
random.seed('123456')
for step in range(nsteps):
    k = random.randrange(N)
    Upsilon = random.uniform(0.0, 1.0)
    h = sum(S[nn] for nn in nbr[k])
    S[k] = -1
    if Upsilon < 1.0 / (1.0 + math.exp(-2.0 * beta * h)):
        S[k] = 1
```

Conclusion

Concepts considered:

- Enumeration (Counting / Listing)
- Metropolis Markov-chain sampling
- Cluster algorithm & a priori probabilities
- Heat-bath algorithm
- Coupling

Algorithms considered:

- enumerate-ising.py (using Gray code)
- thermo-ising.py (using density of states)
- markov-ising.py (Metropolis algorithm)
- cluster-ising.py (Wolff algorithm)
- heat-bath-ising.py (and coupling)

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