Symmetries, Gauge Invariance and Quantization in Discrete Models

Mathematical Modeling and Computational Physics 2009
July 7 - 11, 2009
Joint Institute for Nuclear Research, Dubna, Russia

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July 10, 2009

Motivations and Preliminaries

Discrete systems are widespread in applications

in particular, many nanostructures are symmetric discrete formations

There are many philosophical and physical arguments that discreteness is more suitable for physics at small distances

than continuity which arises only as a logical limit in considering large collections of discrete structures

Subject of our study

- Many important properties of dynamical systems are direct results of their symmetries
- We study deterministic and non-deterministic dynamical systems in discrete time and on discrete lattices with non-trivial symmetries
- As a tool for our study we are developing programs in C based on computer algebra and computational group theory methods

Basic Constituents of Our Models

- Space X is k-valent graph with symmetry group $G = \mathrm{Aut}(X)$ — space symmetries
- Vertices of X take values in the set Σ with symmetry group $\Gamma \leq \mathrm{Sym}\,(\Sigma)$ — internal symmetries
- States of the whole system are functions $\sigma(x) \in \Sigma^X$
- We define whole system symmetry groups W — unifying space G and internal Γ symmetries — as equivalence classes of split extensions $1 \to \Gamma^X \to W \to G \to 1$
- Action of the group W splits the set Σ^X into orbits of different sizes
- Evolution goes in discrete time $t \in \mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\}$
- Dynamics is determined by some evolution rule connecting the current state $\sigma_t(x)$ of the system with its prehistory $\sigma_{t-1}(x),\ \sigma_{t-2}(x),\ \sigma_{t-3}(x), \ldots$

Constructing Whole Symmetry Group W

From space G and internal Γ symmetries

Problem: Combine groups G and Γ acting on X and Σ

into single group W acting on states Σ^X of whole system

Examples: Direct and wreath products

- Direct product $W = \Gamma^X \times G$

$$\begin{aligned} \sigma(x)\,(\alpha\,(x),\ a) &= \sigma\,(x)\,\alpha\,(x) && \textit{action on } \Sigma^X \\ (\alpha\,(x),\ a) * (\beta\,(x),\ b) &= (\alpha\,(x)\,\beta\,(x),\ ab) && \textit{multiplication rule} \end{aligned}$$

- Wreath product $W = \Gamma \wr_X G \cong \Gamma^X \rtimes G$

$$\begin{aligned} \sigma(x)\,(\alpha\,(x),\ a) &= \sigma\left(xa^{-1}\right)\alpha\left(xa^{-1}\right) \\ (\alpha\,(x),\ a) * (\beta\,(x),\ b) &= (\alpha\,(x)\,\beta\,(xa),\ ab) \end{aligned}$$

Generalizing Statement

There are equivalence classes of group multiplications providing Cartesian product $\Gamma^X \otimes G$ *with structure of semidirect product* $\Gamma^X \rtimes G$

Equivalence classes are given by antihomomorphisms $\mu : G \to G$

Equivalence relations are described by arbitrary functions $\kappa : G \to G$

Group operations:

- *Action on* Σ^X*:* $\sigma(x)\,(\alpha\,(x),\ a) \ = \ \sigma\,(x\mu(a))\,\alpha\,(x\kappa(a))$
- *Multiplication:* $(\alpha\,(x),\ a) * (\beta\,(x),\ b)$
$$= \left(\alpha\left(x\kappa(ab)^{-1}\mu(b)\kappa(a)\right)\beta\left(x\kappa(ab)^{-1}\kappa(b)\right),\ ab\right)$$
- *Inverse element:*
$$(\alpha(x),\ a)^{-1} = \left(\alpha\left(x\kappa\left(a^{-1}\right)^{-1}\mu(a)^{-1}\kappa(a)\right)^{-1},\ a^{-1}\right)$$

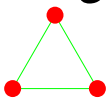
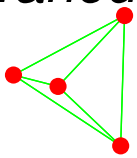
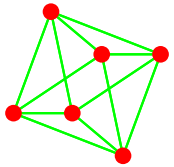
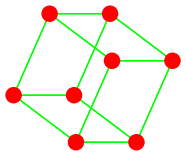
Standard products are obtained by fixing

$$\begin{cases} \mu(a) = 1, \quad \kappa(a) = 1 & \longrightarrow \quad \text{direct product} \\ \mu(a) = a^{-1},\ \kappa(a) = a^{-1}\ (\text{or } \kappa(a) = 1\ ) & \longrightarrow \quad \text{wreath product} \end{cases}$$

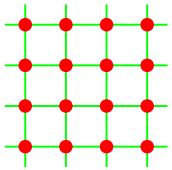
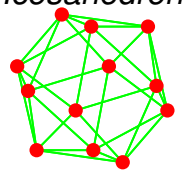
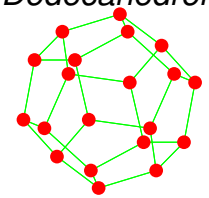
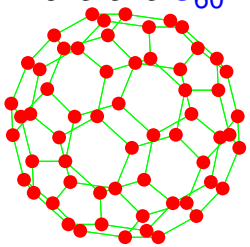
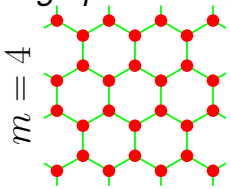
For Models with Locally Defined Evolution Rules the group of local symmetries G_{loc} is essential

- G_{loc} is subgroup of the space group: $G_{loc} \leq G$
- G_{loc} is symmetry group of neighborhood of any vertex x_i from X
- G_{loc} is the stabilizer of x_i: $g \in G_{loc} = \mathrm{Stab}_G(x_i)$ means $x_i g = x_i$
- Evolution rules of such models are reduced to local rules
- Local rules are defined on orbits of G_{loc} on edges from the vertex neighborhoods
- Typical examples of models with locally defined evolution rules are cellular automata and Ising model
- Later we will introduce also local quantum models on regular graphs

Examples of Discrete Spaces. I

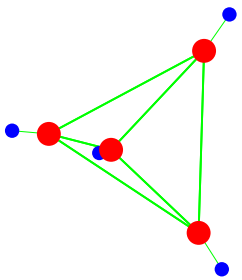
X	N_X	N_E	G	$\lvert G\rvert$
Atom	1	0	1	1
Dimer	2	1	$\mathrm{Sym}\,(2) \cong \mathbb{Z}_2$	2
Triangle 	3	3	$\mathrm{Sym}\,(3) \cong \mathrm{D}_6$	6
n-*vertex polygon*	n	n	D_{2n}	$2n$
Tetrahedron 	4	6	$\mathrm{Sym}\,(4)$	24
Octahedron 	6	12	$\mathbb{Z}_2 \times \mathrm{Sym}\,(4)$	48
Hexahedron 	8	12	$\mathbb{Z}_2 \times \mathrm{Sym}\,(4)$	48

Examples of Discrete Spaces. II

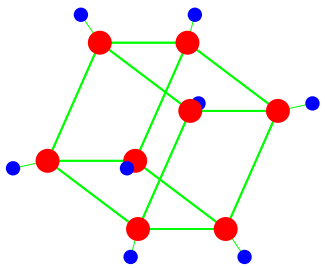
X	N_X	N_E	G	$\lvert G\rvert$
Toric square $n\times n$, $n\neq 4$	n^2	$2n^2$	$(\mathbb{Z}_n \times \mathbb{Z}_n) \rtimes \mathrm{D}_8$	$8n^2$
$n = 4$ 	16	32	$((((\mathbb{Z}_2 \times \mathrm{D}_8) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_3) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_2$	384
Icosahedron 	12	30	$\mathbb{Z}_2 \times \mathrm{Alt}(5)$	120
Dodecahedron 	20	30	$\mathbb{Z}_2 \times \mathrm{Alt}(5)$	120
Fullerene C_{60} 	60	90	$\mathbb{Z}_2 \times \mathrm{Alt}(5)$	120
Toric graphene $n\times m$ 	nm	$\frac{3nm}{2}$	$\mathrm{D}_n \times \mathrm{D}_{2m}$	$2nm$

Symmetries of 3-valent (Hydro)Carbon Nanostructures

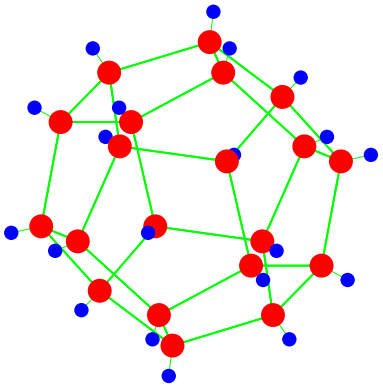
Tetrahedrane C_4H_4
$G = \mathrm{Sym}(4)$
$G_{loc} = \mathrm{D}_6 \cong \mathrm{Sym}(3)$



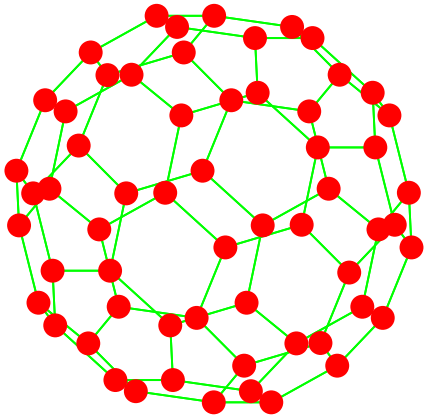
Cubane C_8H_8
$G = \mathbb{Z}_2 \times \mathrm{Sym}(4)$
$G_{loc} = \mathrm{D}_6$



Dodecahedrane $C_{20}H_{20}$
$G = \mathbb{Z}_2 \times \mathrm{Alt}(5)$
$G_{loc} = \mathrm{D}_6$



Fullerene C_{60}
$G = \mathbb{Z}_2 \times \mathrm{Alt}(5)$
$G_{loc} = \mathbb{Z}_2$



Toric graphene $n \times m$

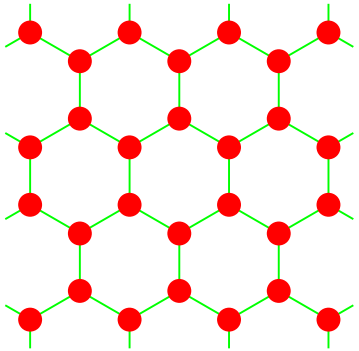
$G = \mathrm{D}_n \times \mathrm{D}_{2m}$
$G_{loc} = \mathbb{Z}_2$

$n, m \to \infty$

$G = (\mathbb{Z} \times \mathbb{Z}) \rtimes \mathrm{D}_6$
$G_{loc} = \mathrm{D}_6$

$n = 6$

$m = 4$



Deterministic and Non-deterministic Models

- Evolution rule of deterministic (or causal) dynamical system

is functional relation — current state is function of prehistory:

$$\sigma_t(x) = F(\sigma_{t-1}(x), \sigma_{t-2}(x), \sigma_{t-3}(x), \ldots)$$

Cellular automaton is typical example

- Dynamical trajectories of deterministic system pass group orbits in non-decreasing order of sizes
- Periodic trajectories lie within orbits of the same size

- Mesoscopic lattice model is a sort of Markov chain

— transition from one state to any other is possible with probability controlled by a Hamiltonian

- Quantum system

— probabilities of transitions between states are squares of complex-valued transition amplitudes

Formation of Soliton-like Structures in Deterministic Dynamics

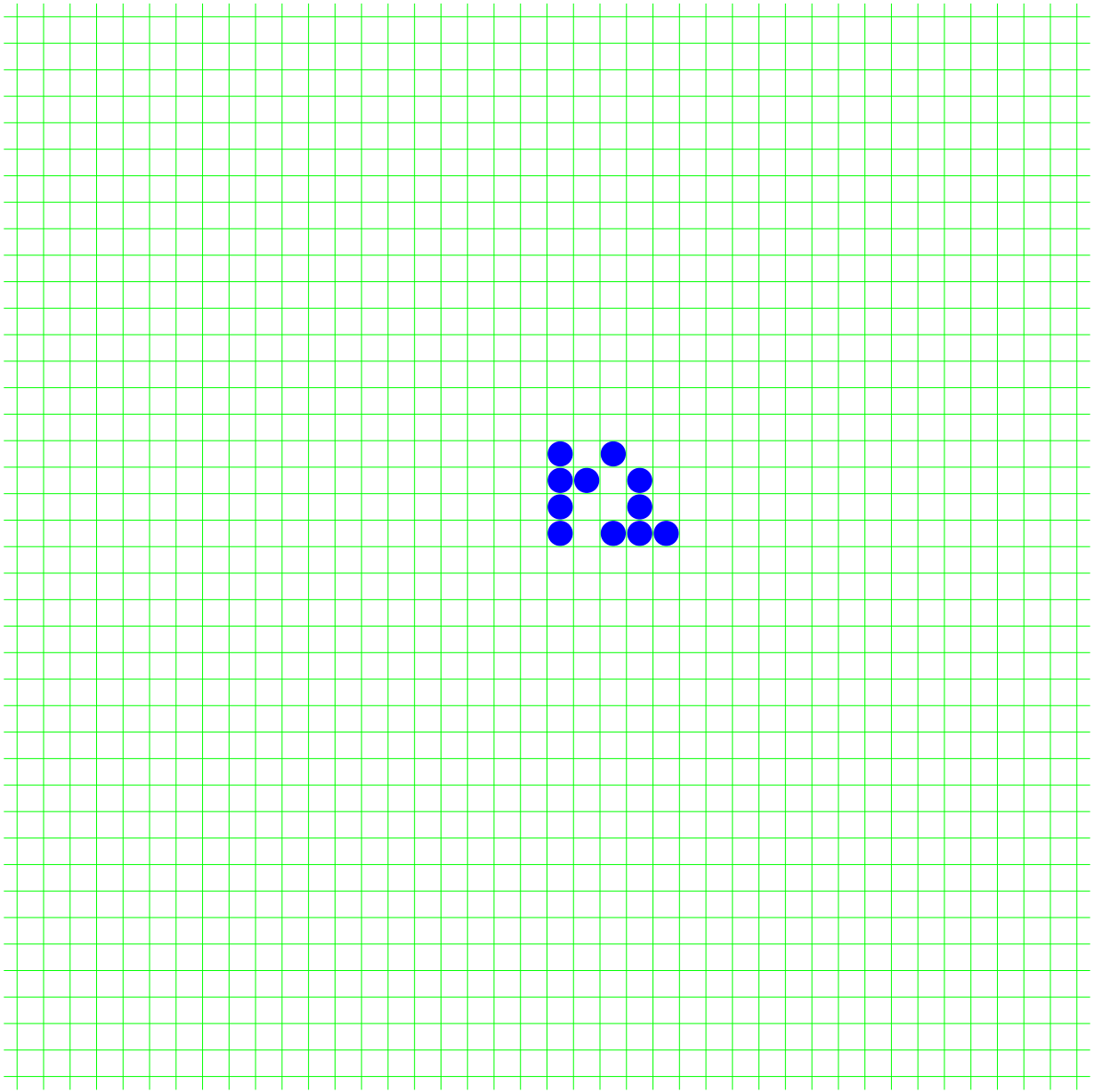
For deterministic dynamics recurrence of trajectory to the same orbit is typical

In such a case the evolution $\sigma_{t_0}(x) \to \sigma_{t_1}(x) = A_{t_1 t_0}(\sigma_{t_0}(x))$ can be replaced by the group action $\sigma_{t_1}(x) = w\sigma_{t_0}(x), \quad w \in W$, i.e., the initial state $\sigma_{t_0}(x)$ is reproduced after some "movement" in the space of states Σ^X.

Examples:

- running waves $\sigma(x - vt)$ in mathematical physics — Galilei group
- "generalized coherent states" in quantum physics — unitary representations of Lie groups
- "spaceships" in cellular automata — lattice symmetries

Example of “spaceship”: “Glider” in Conway’s “Game of Life”



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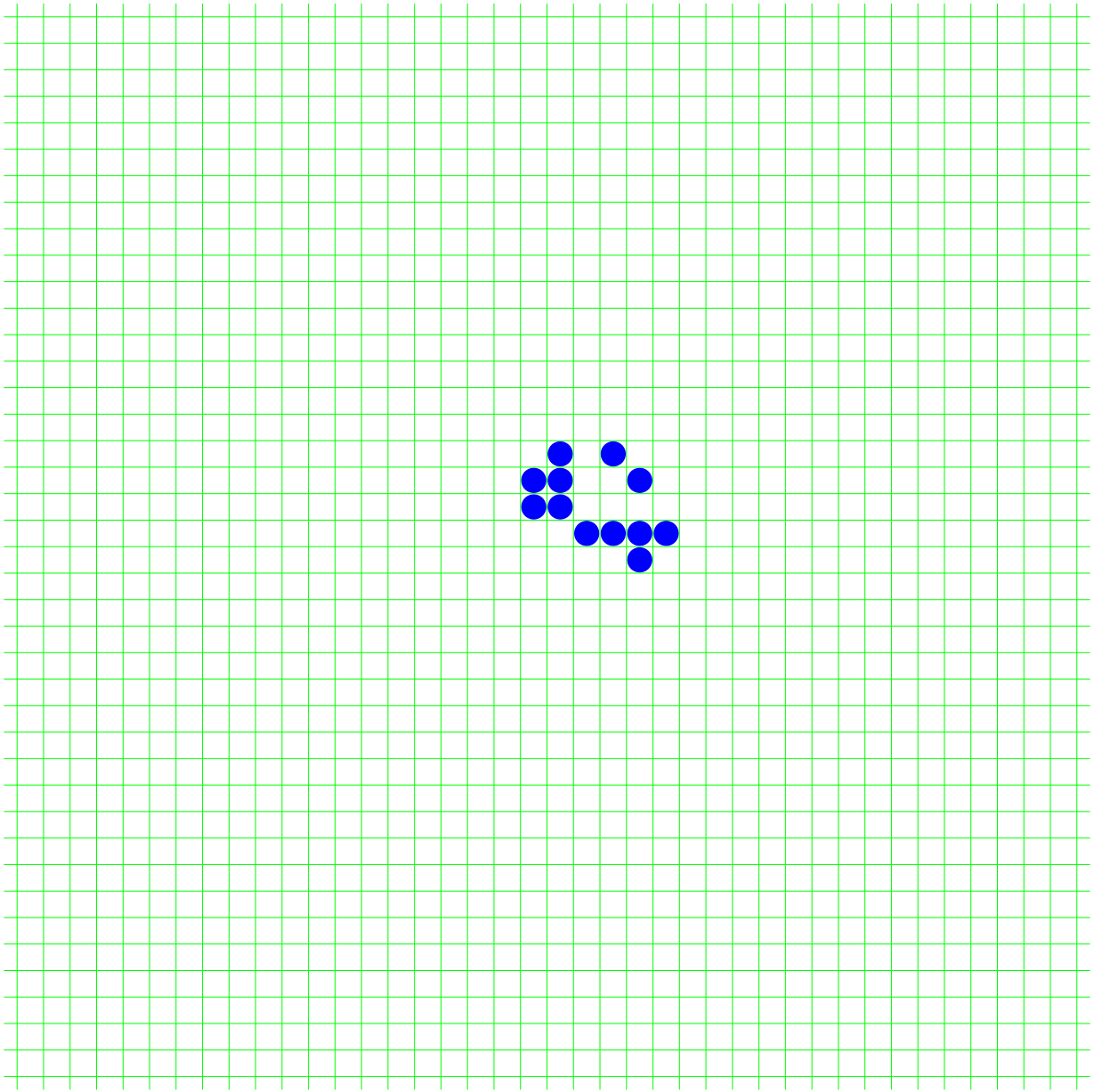

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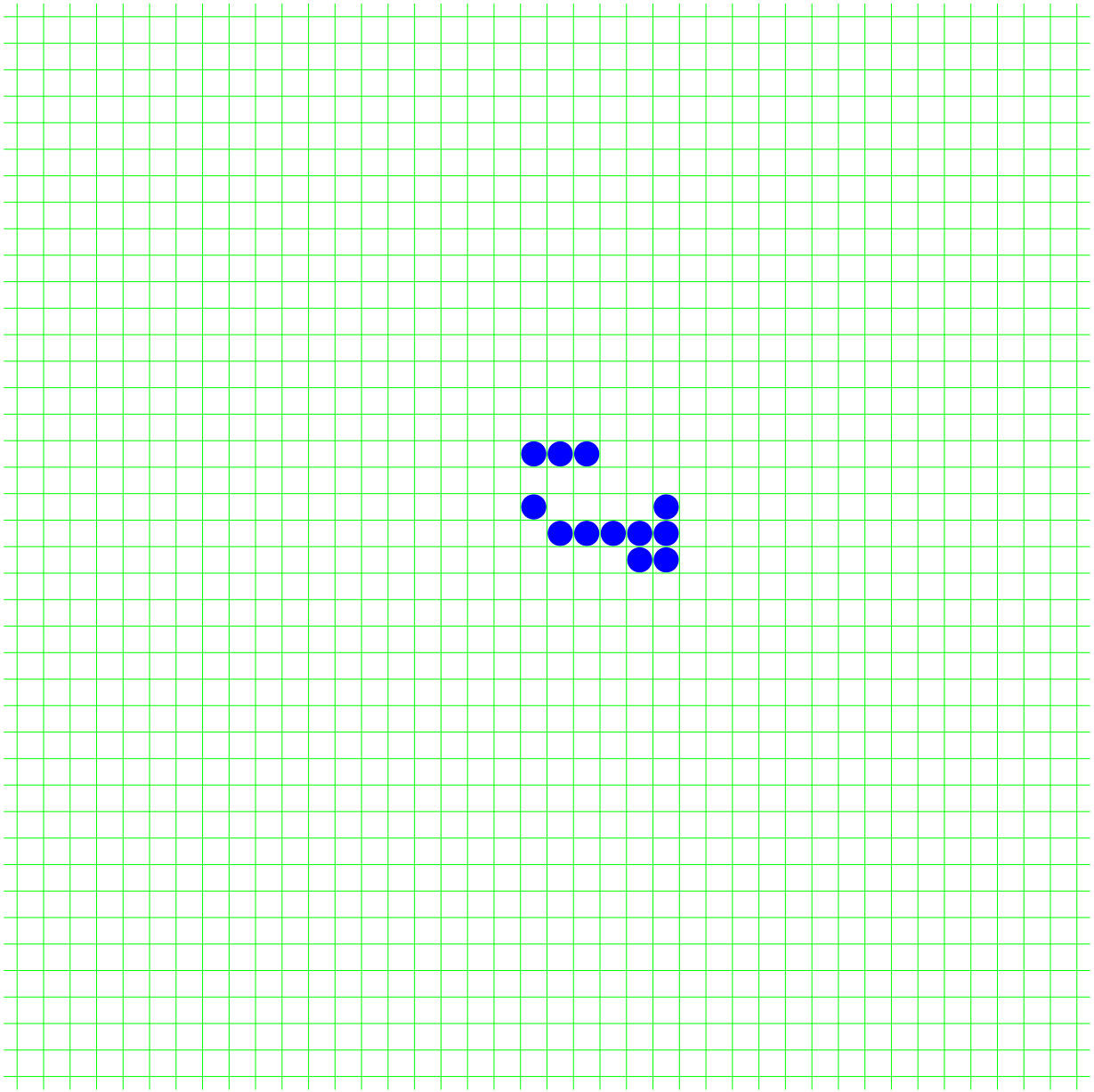

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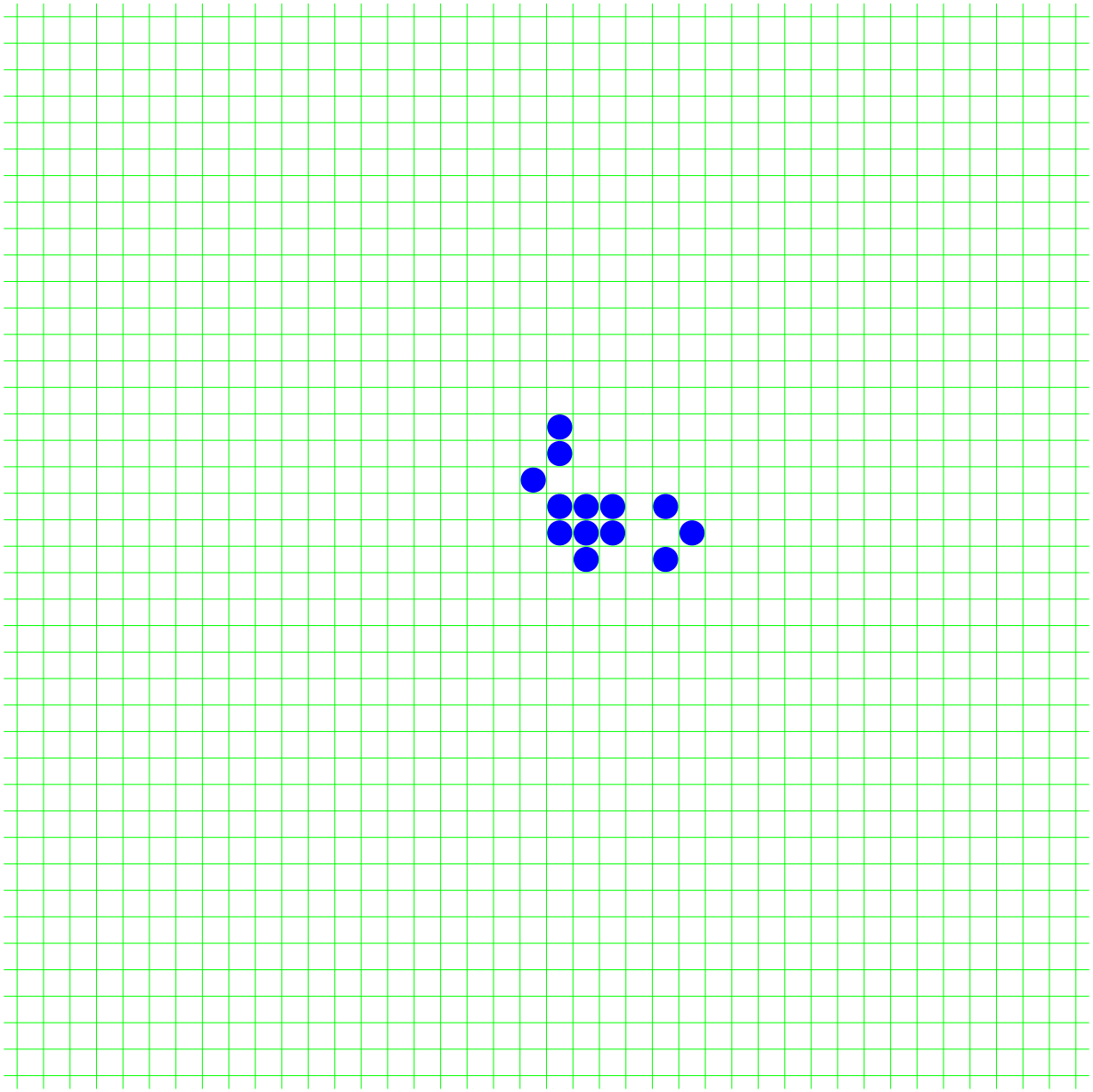

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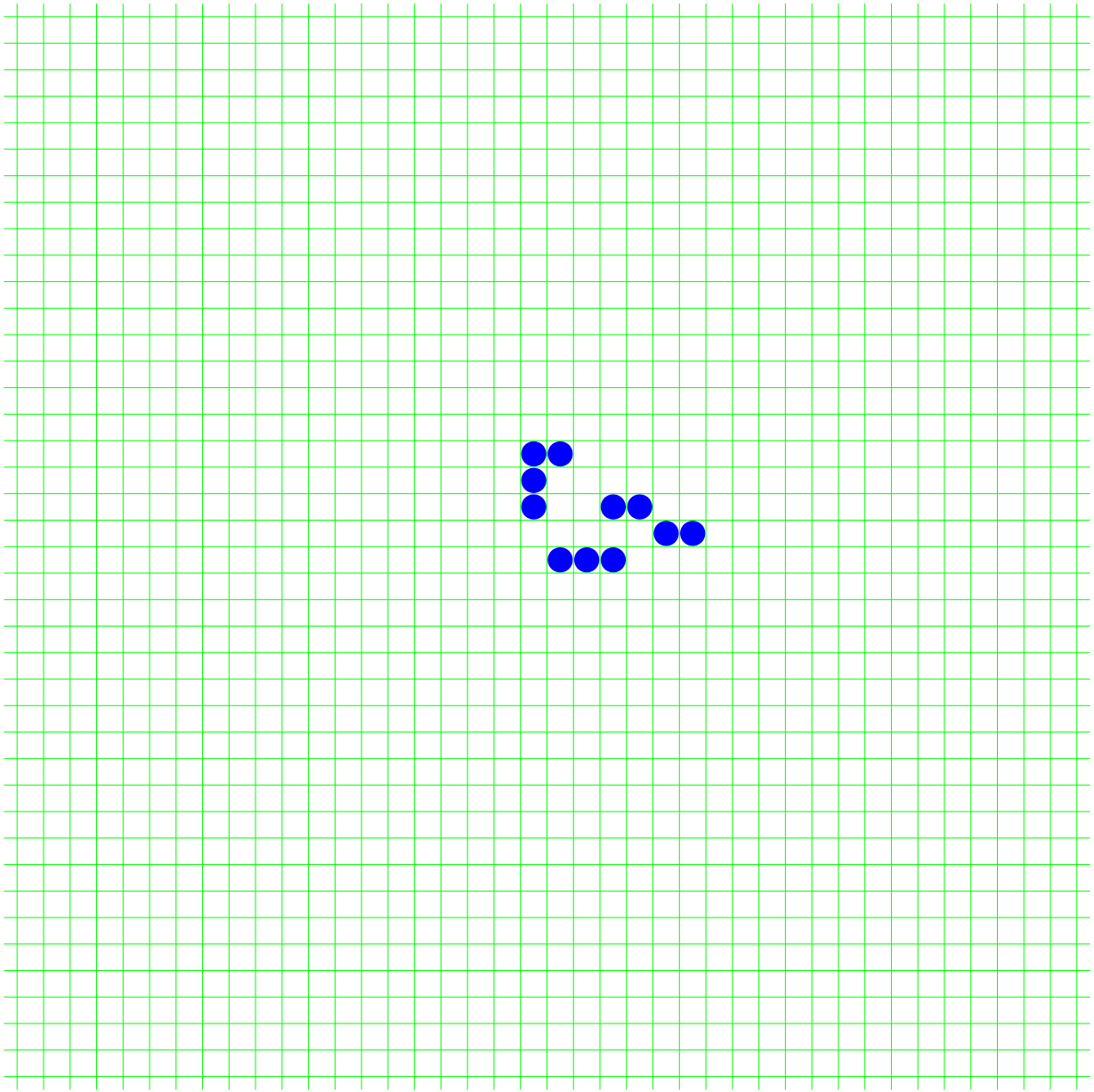

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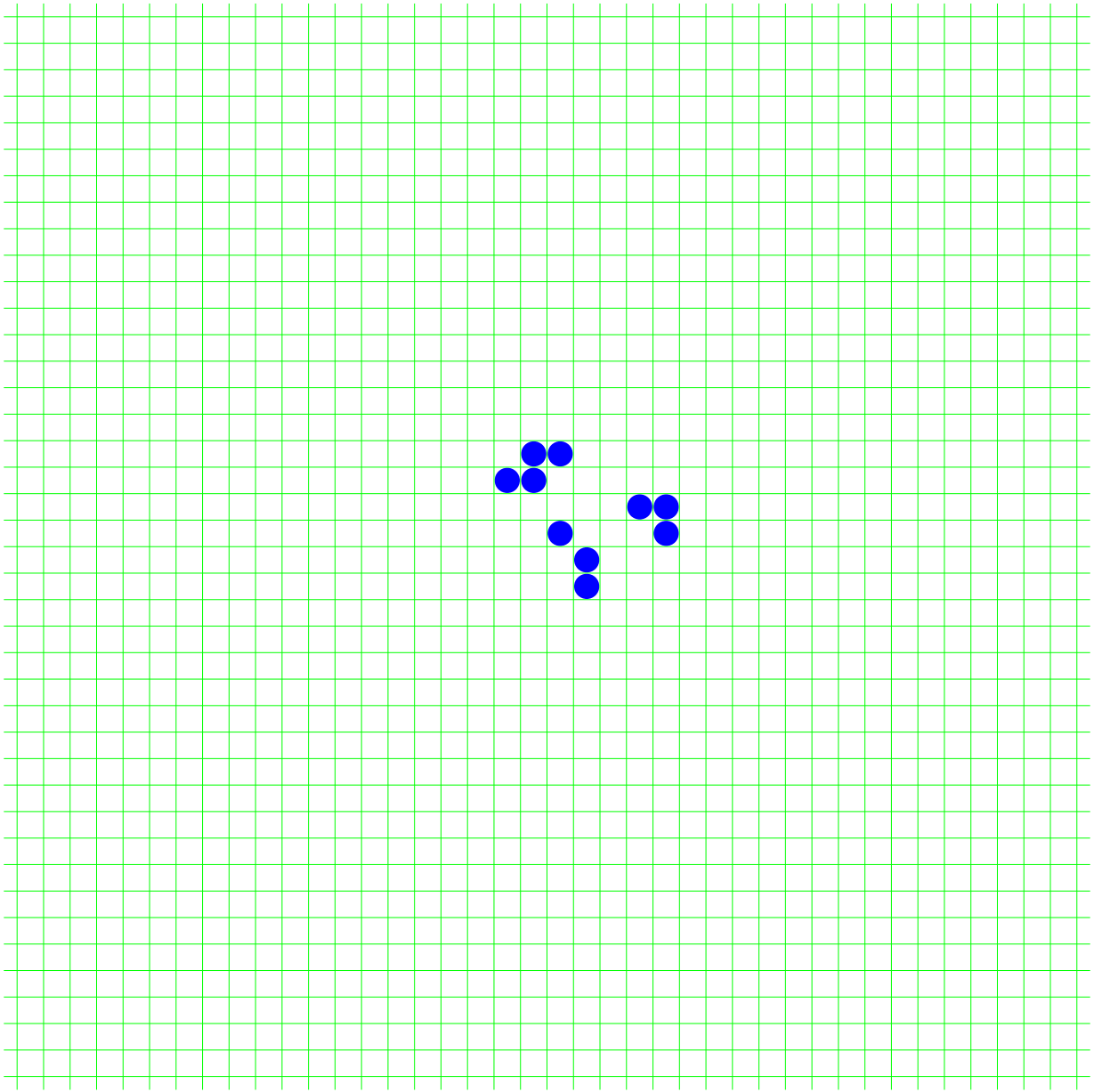

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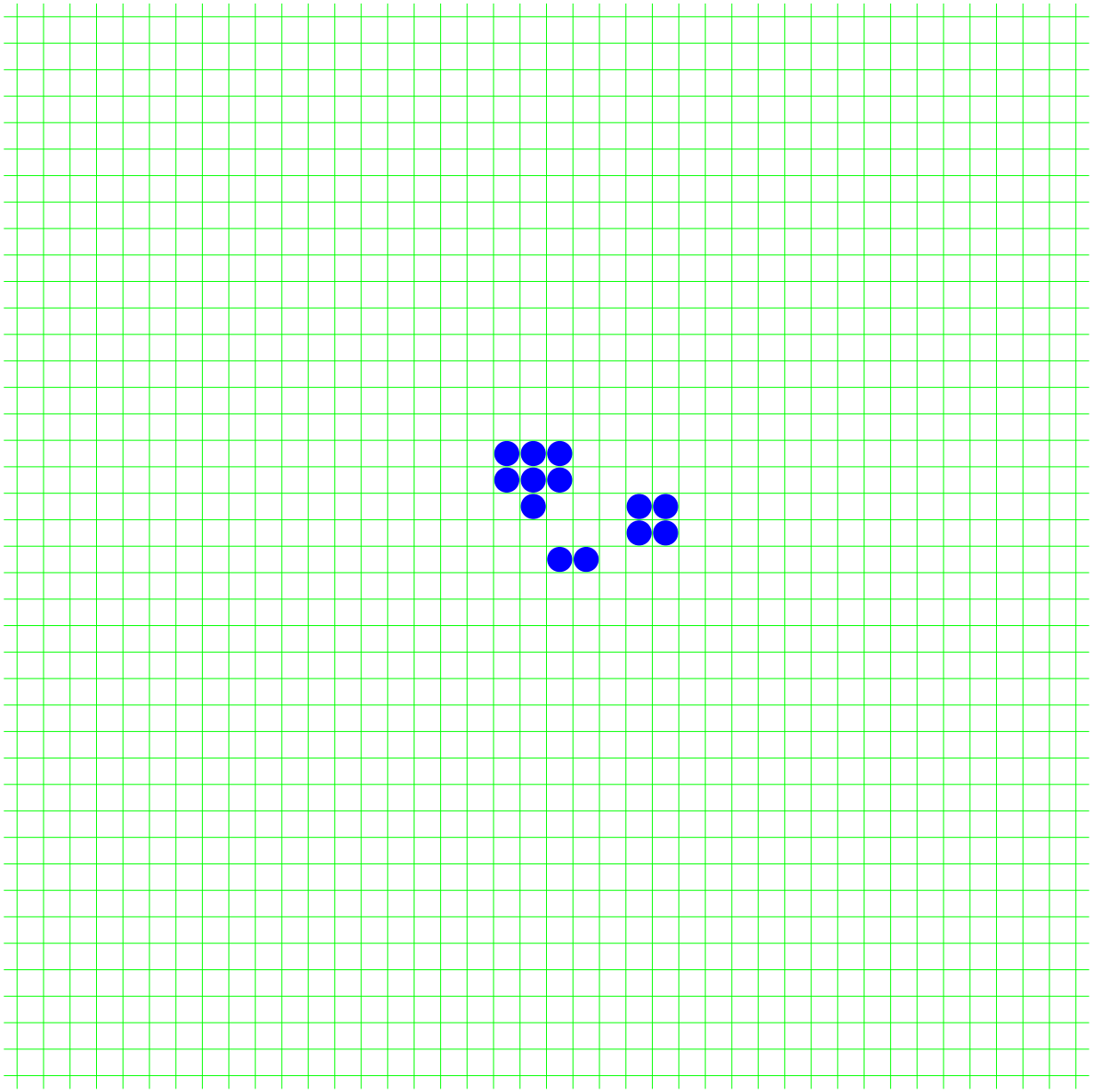

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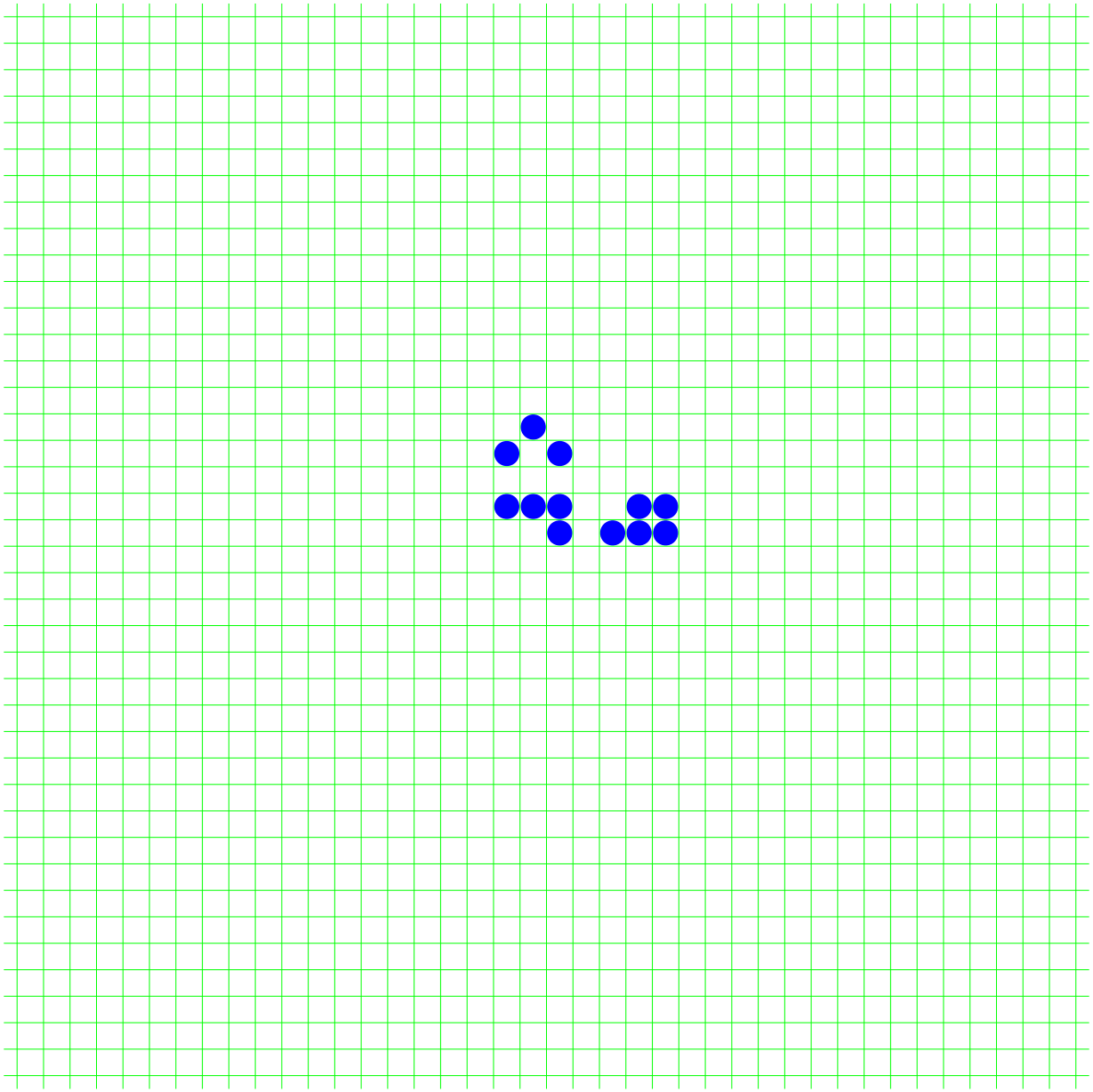

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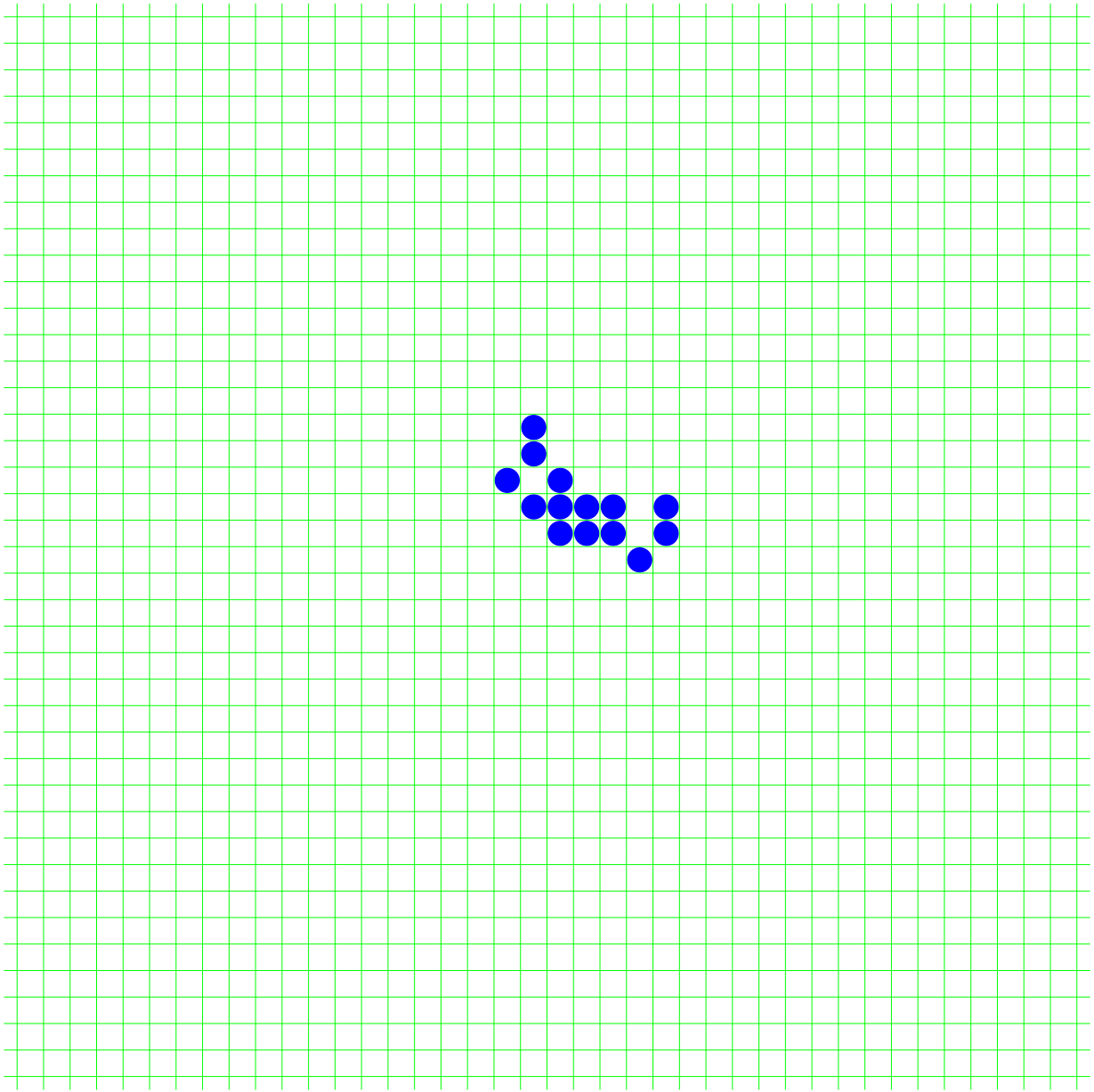

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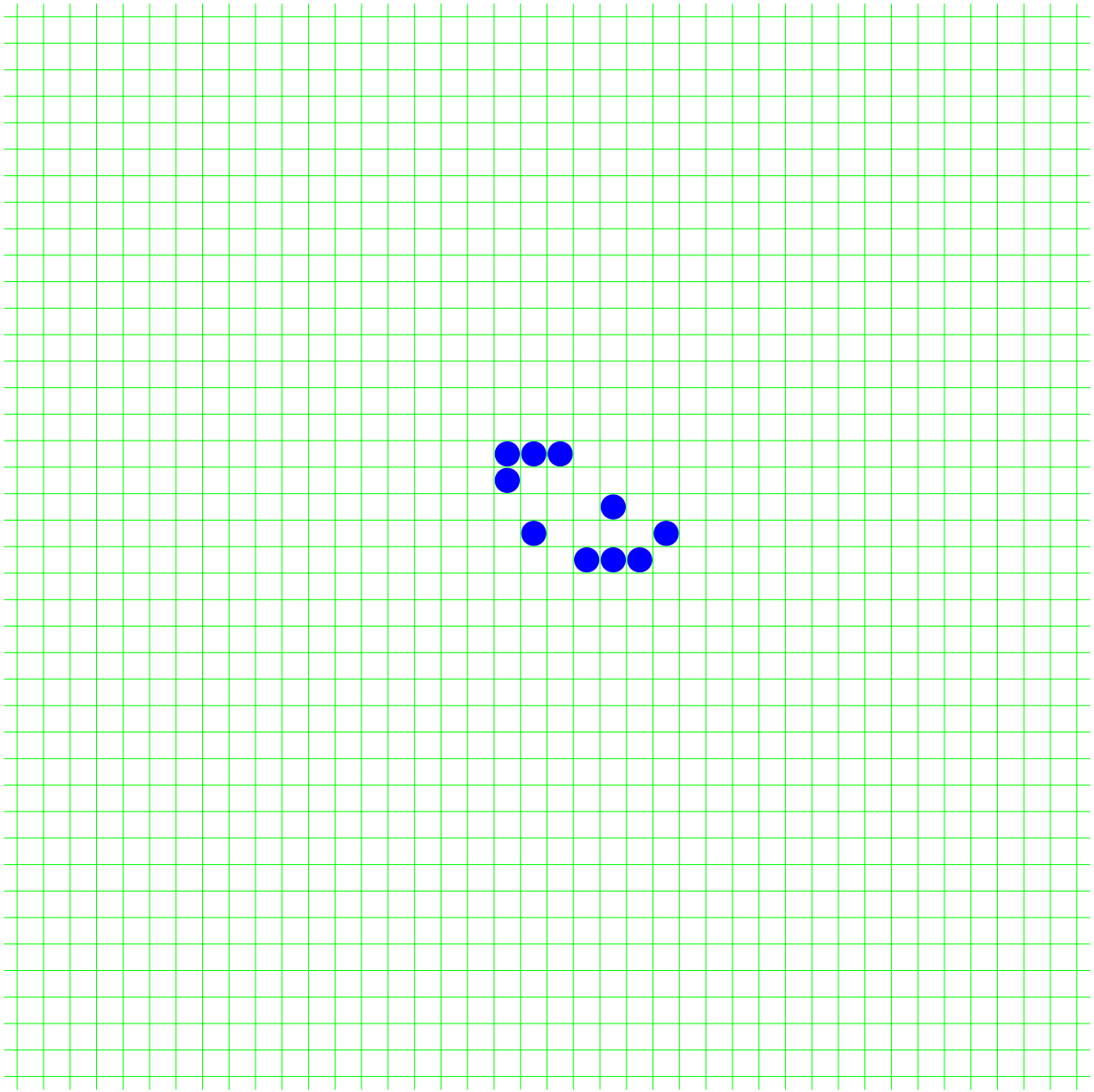

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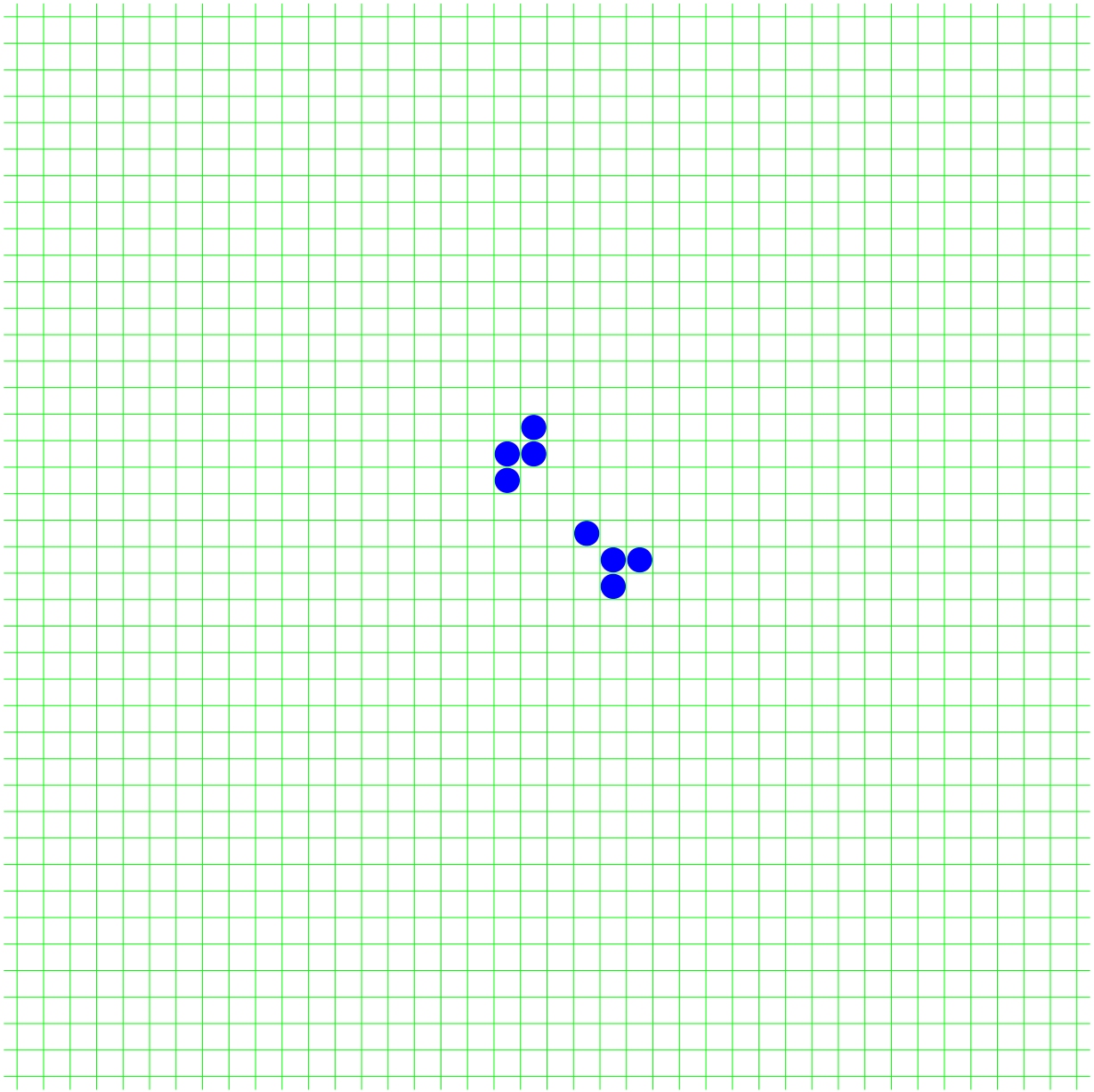

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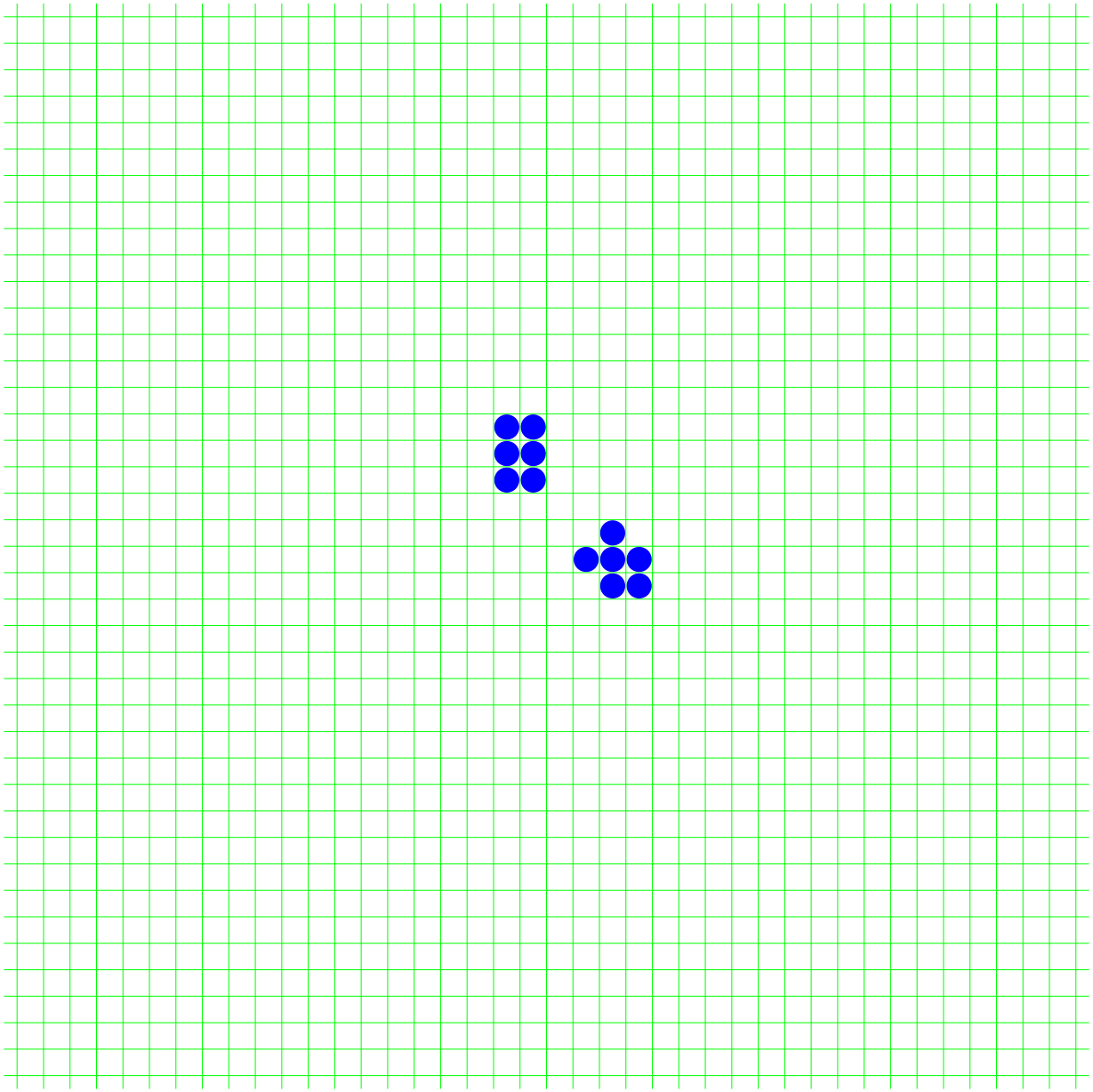

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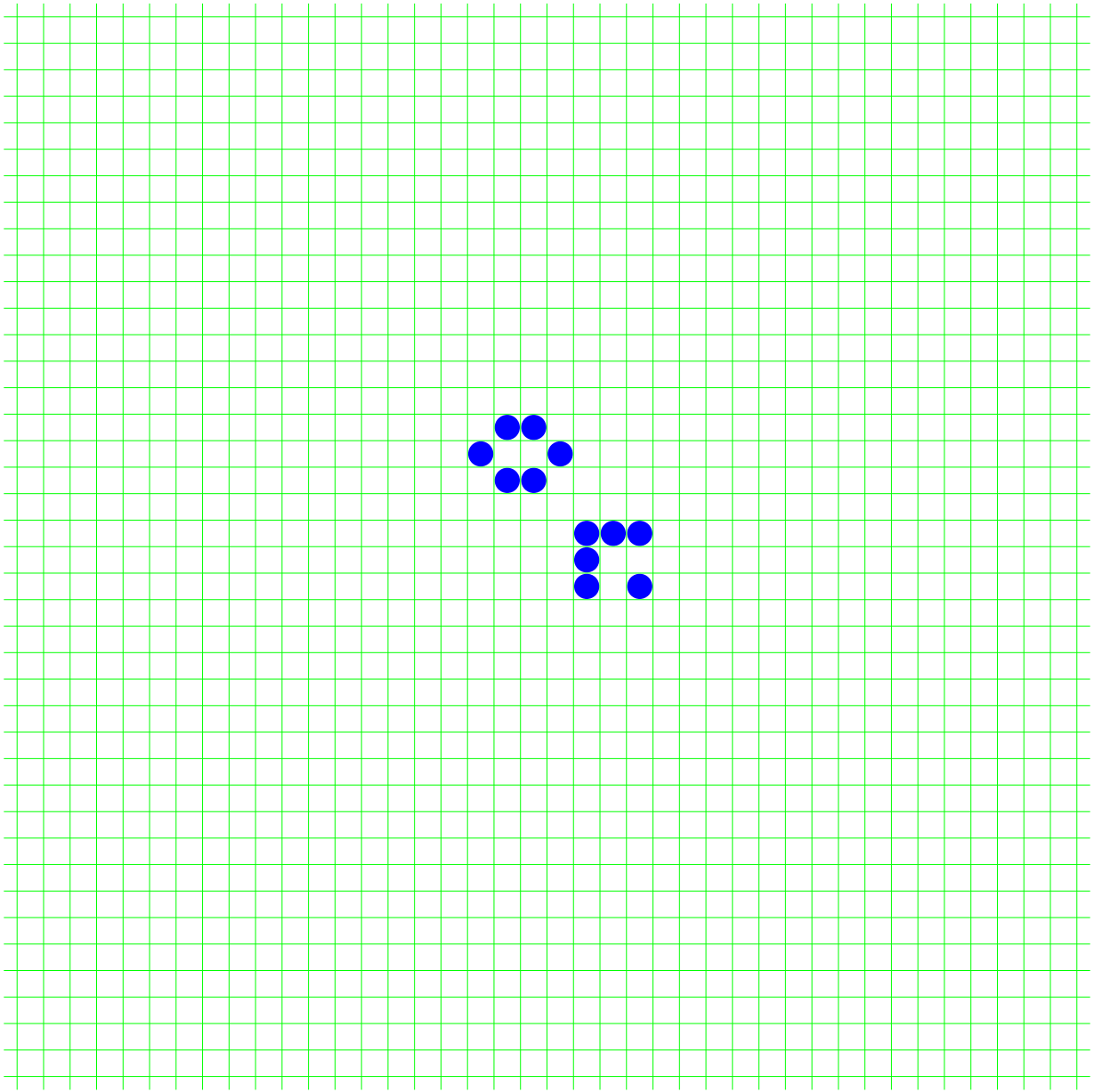

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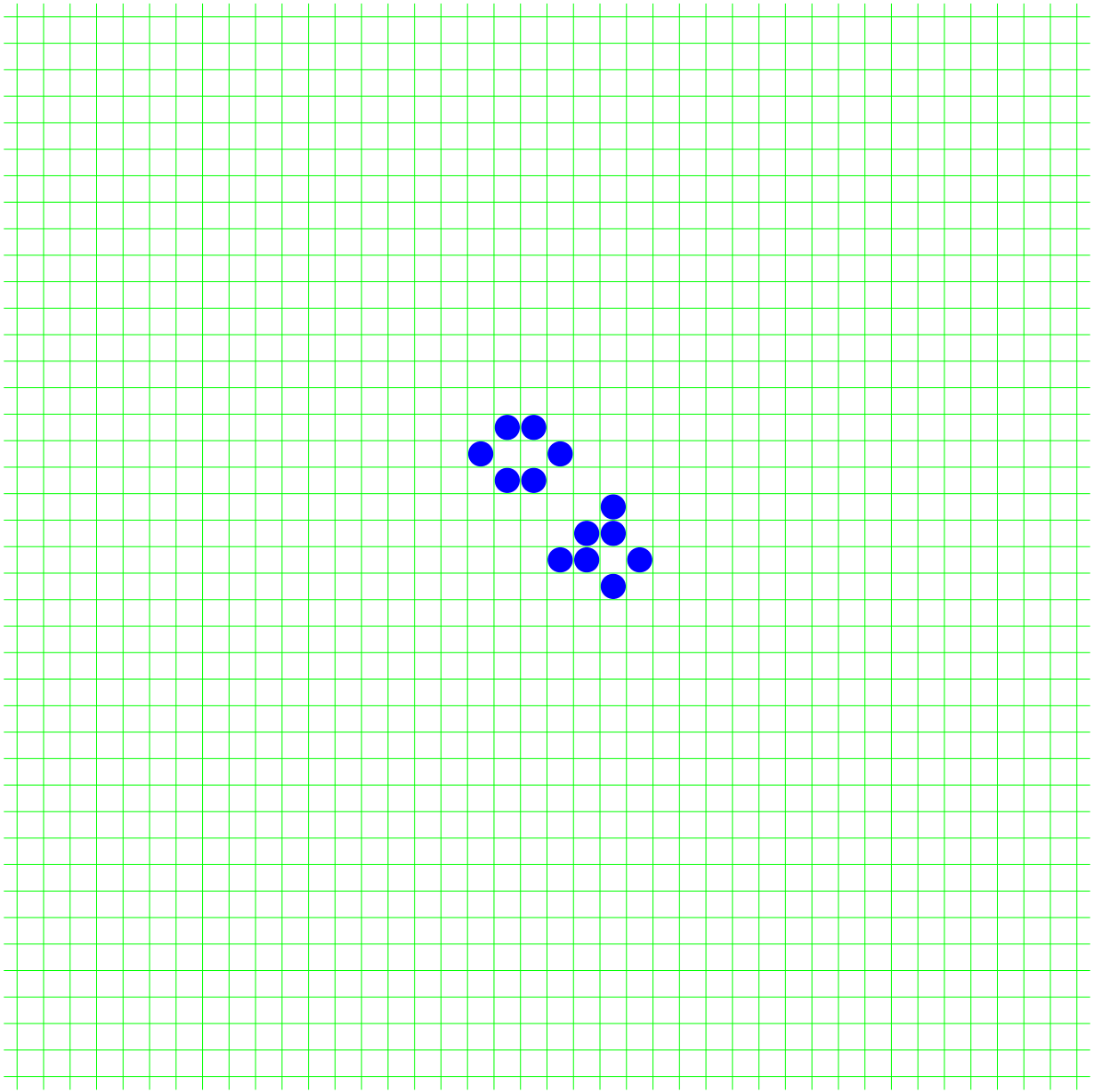

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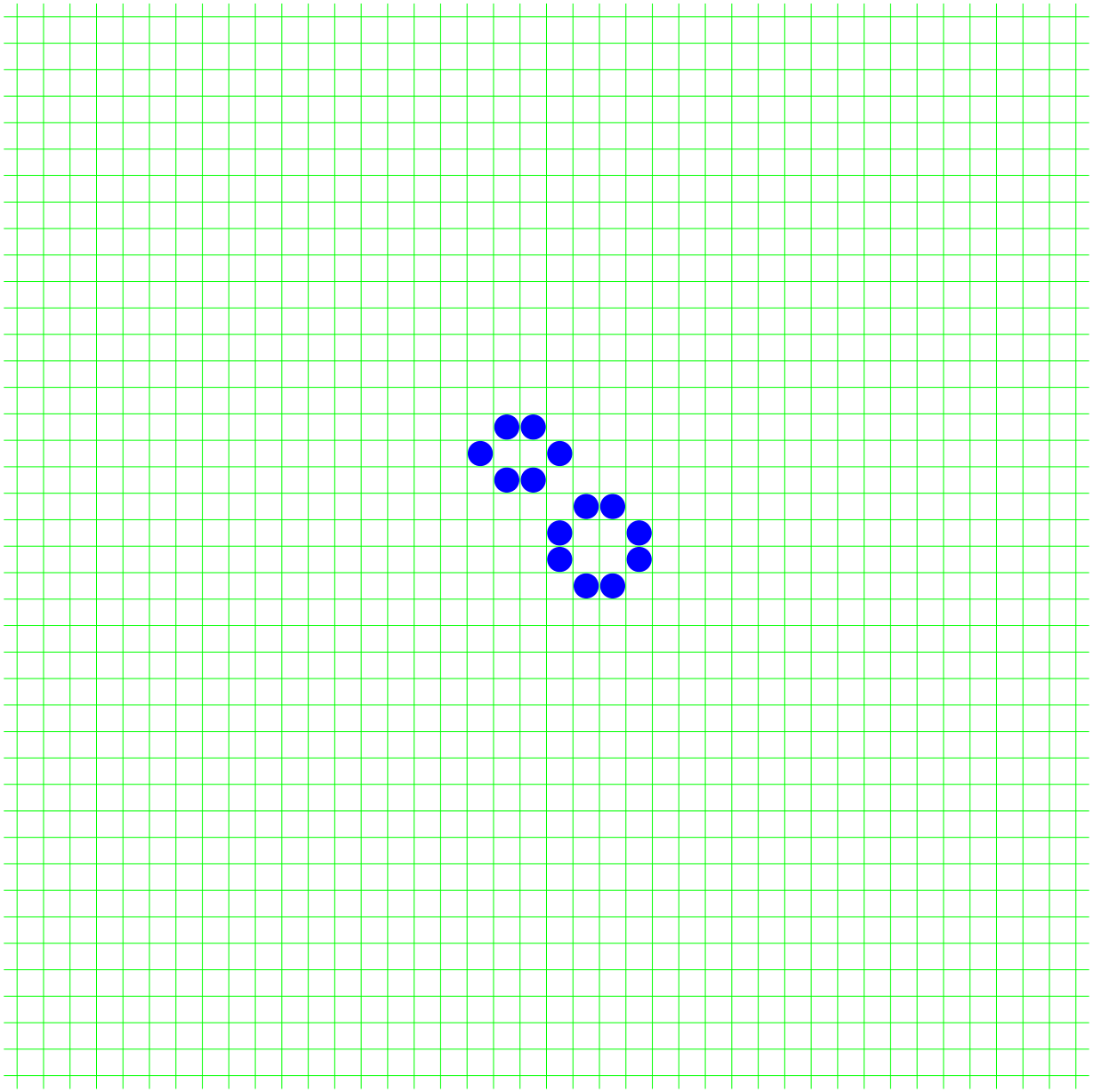

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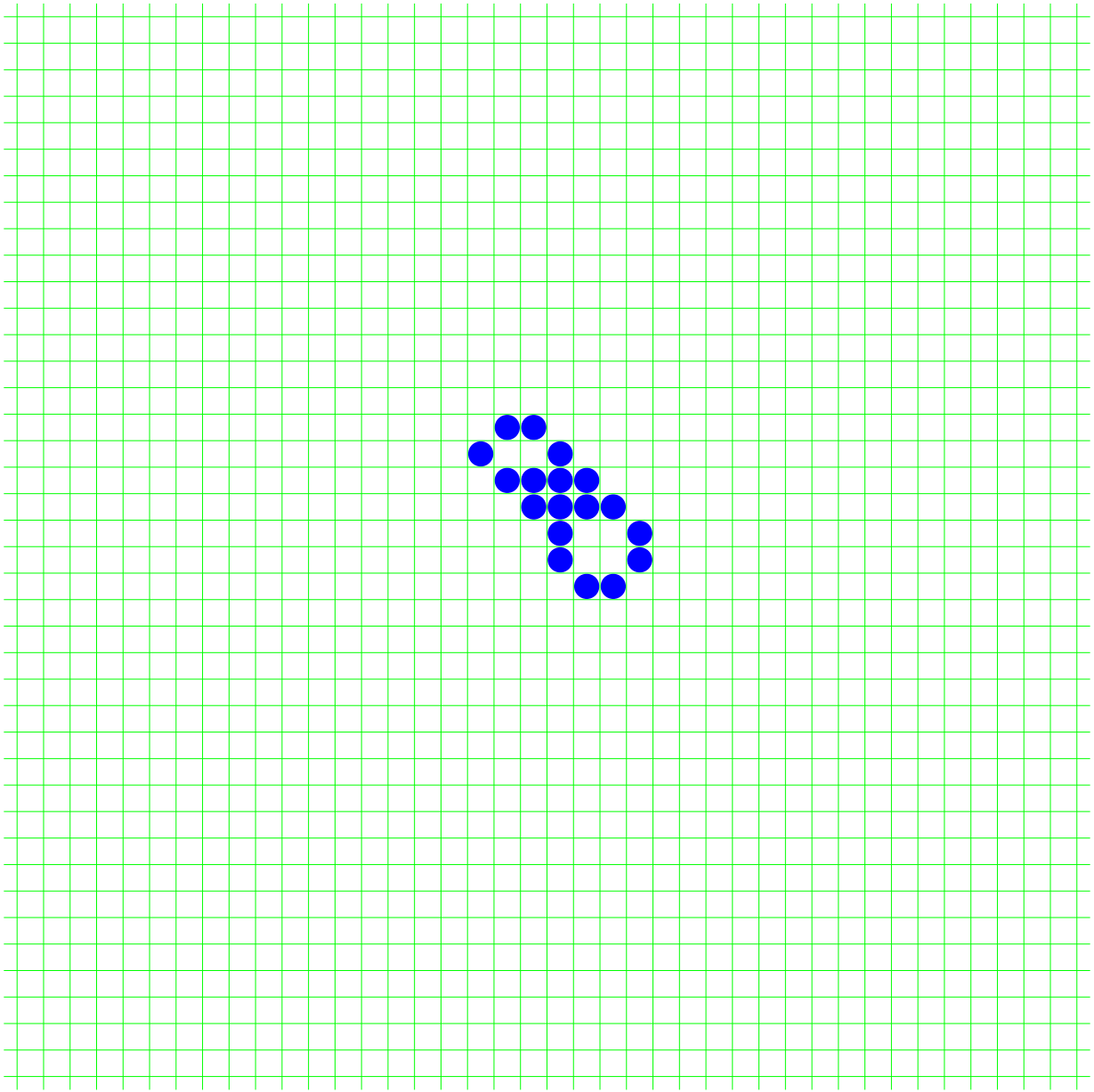

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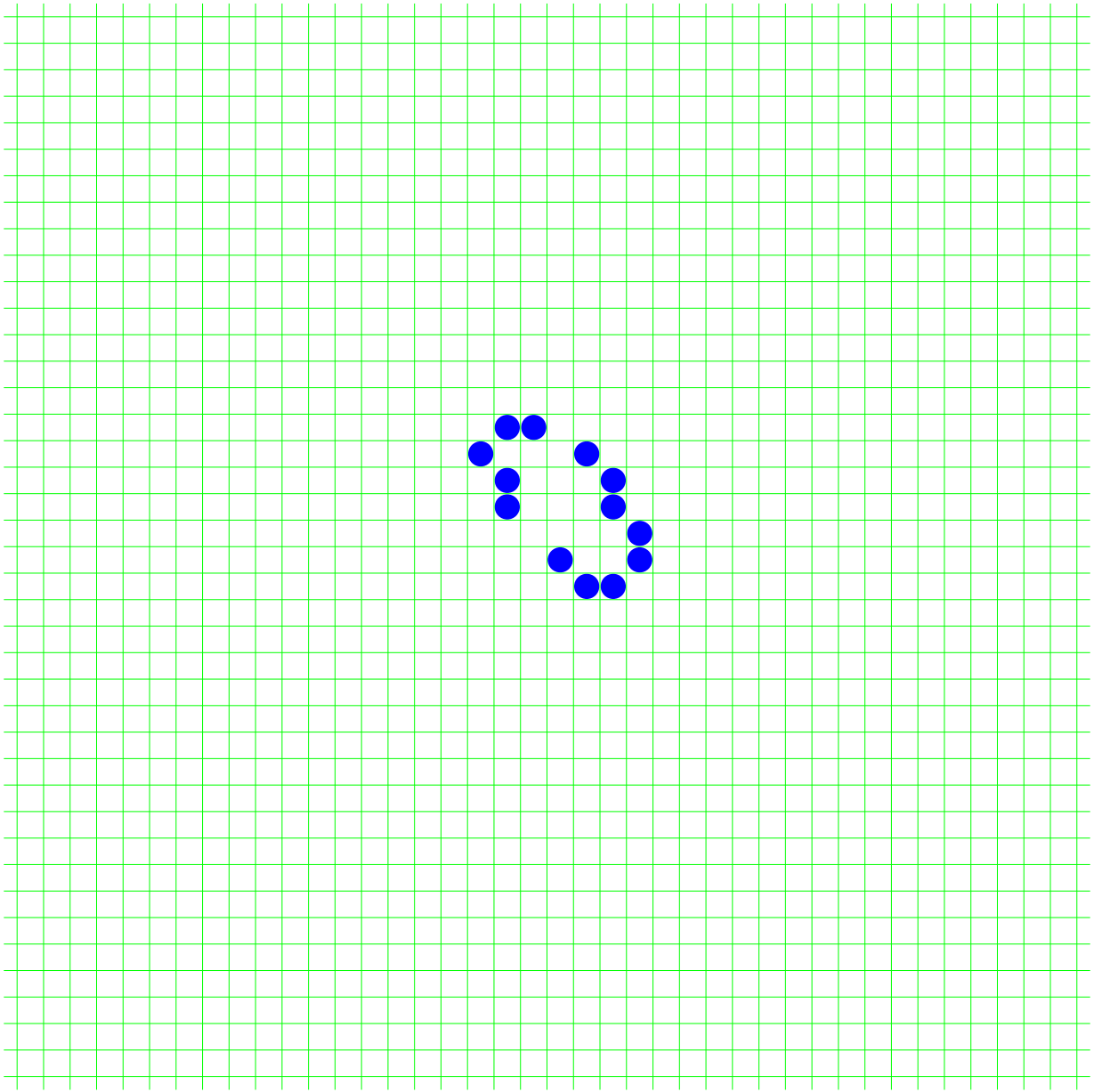

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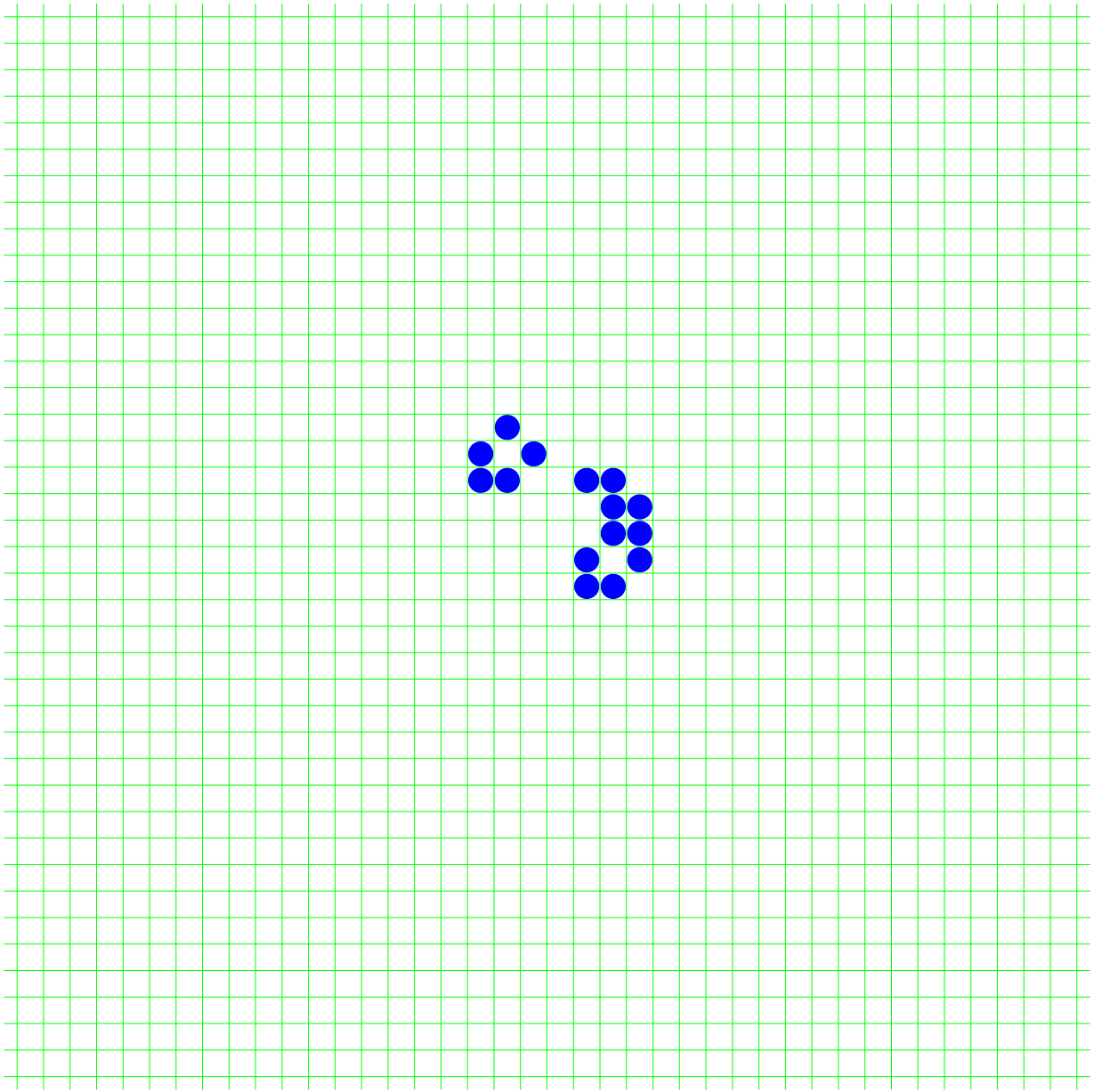

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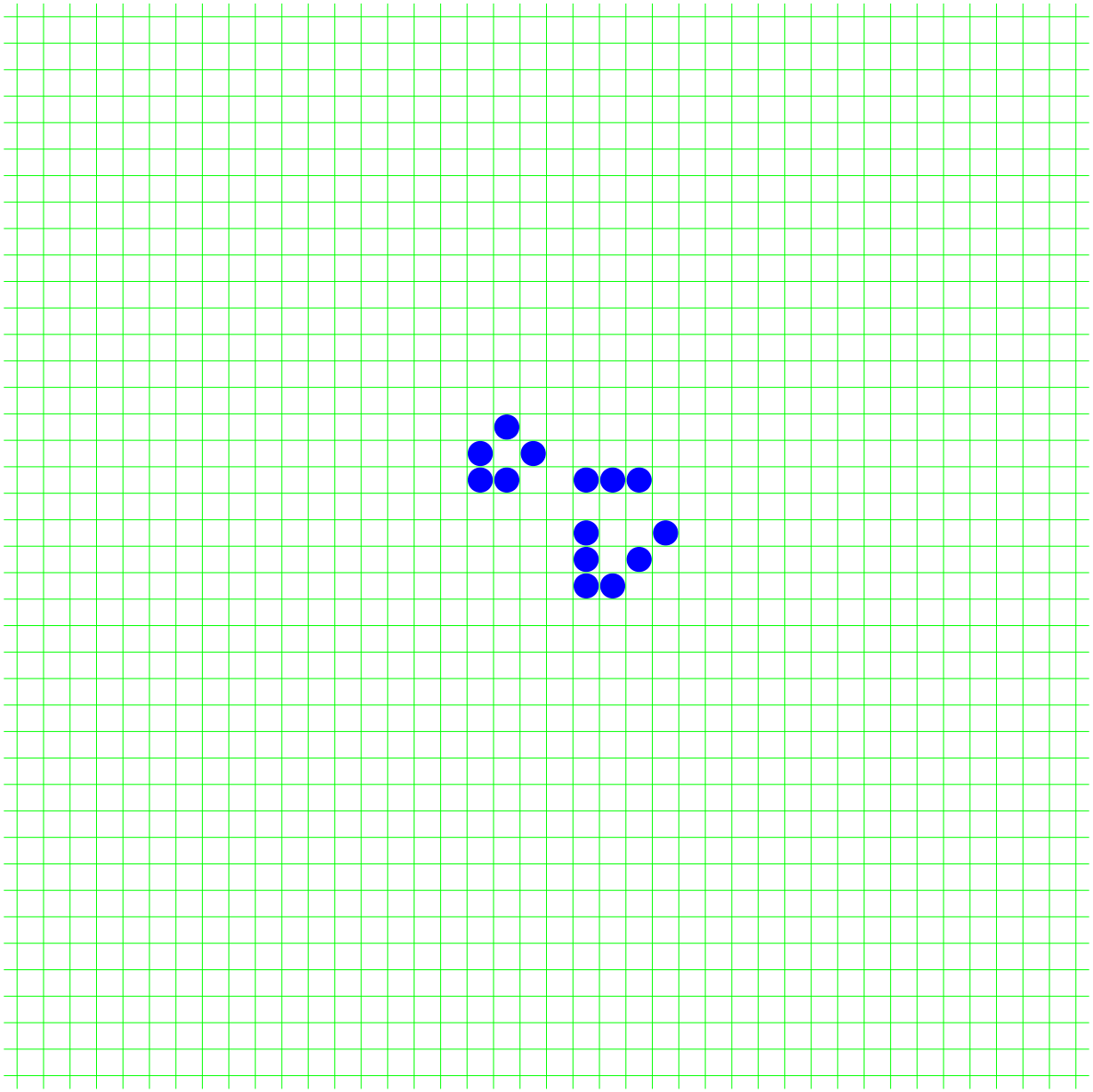

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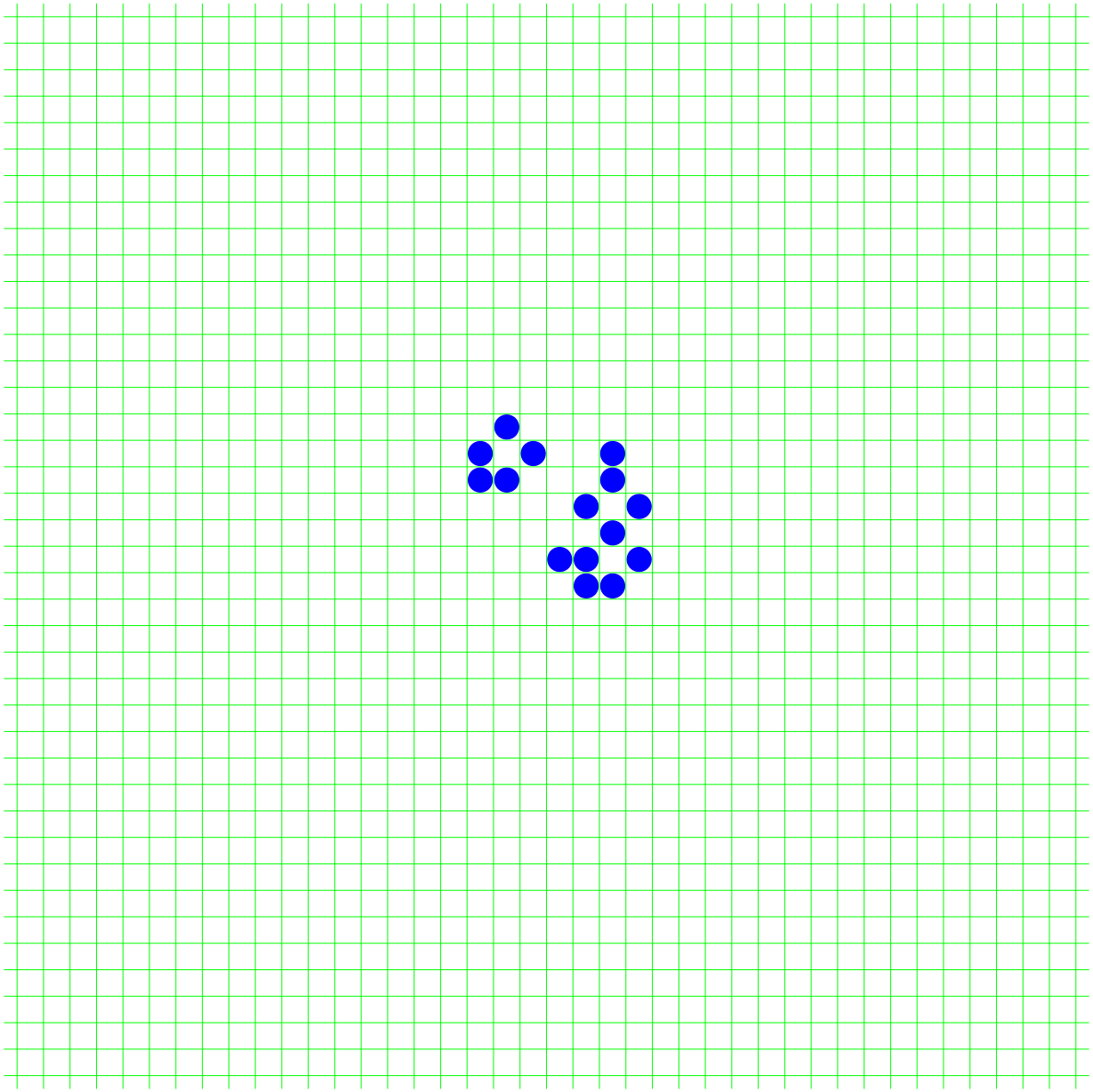

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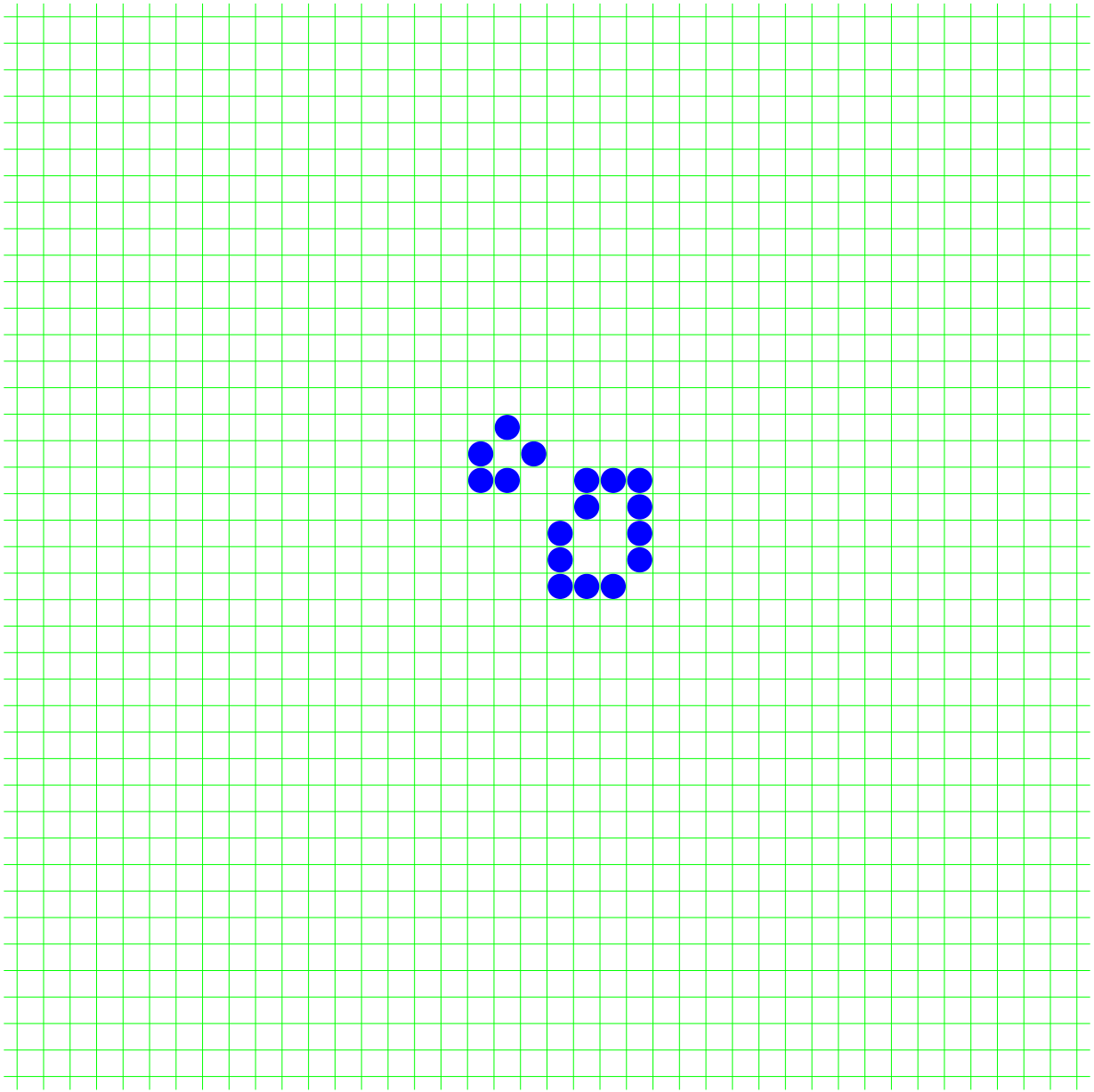

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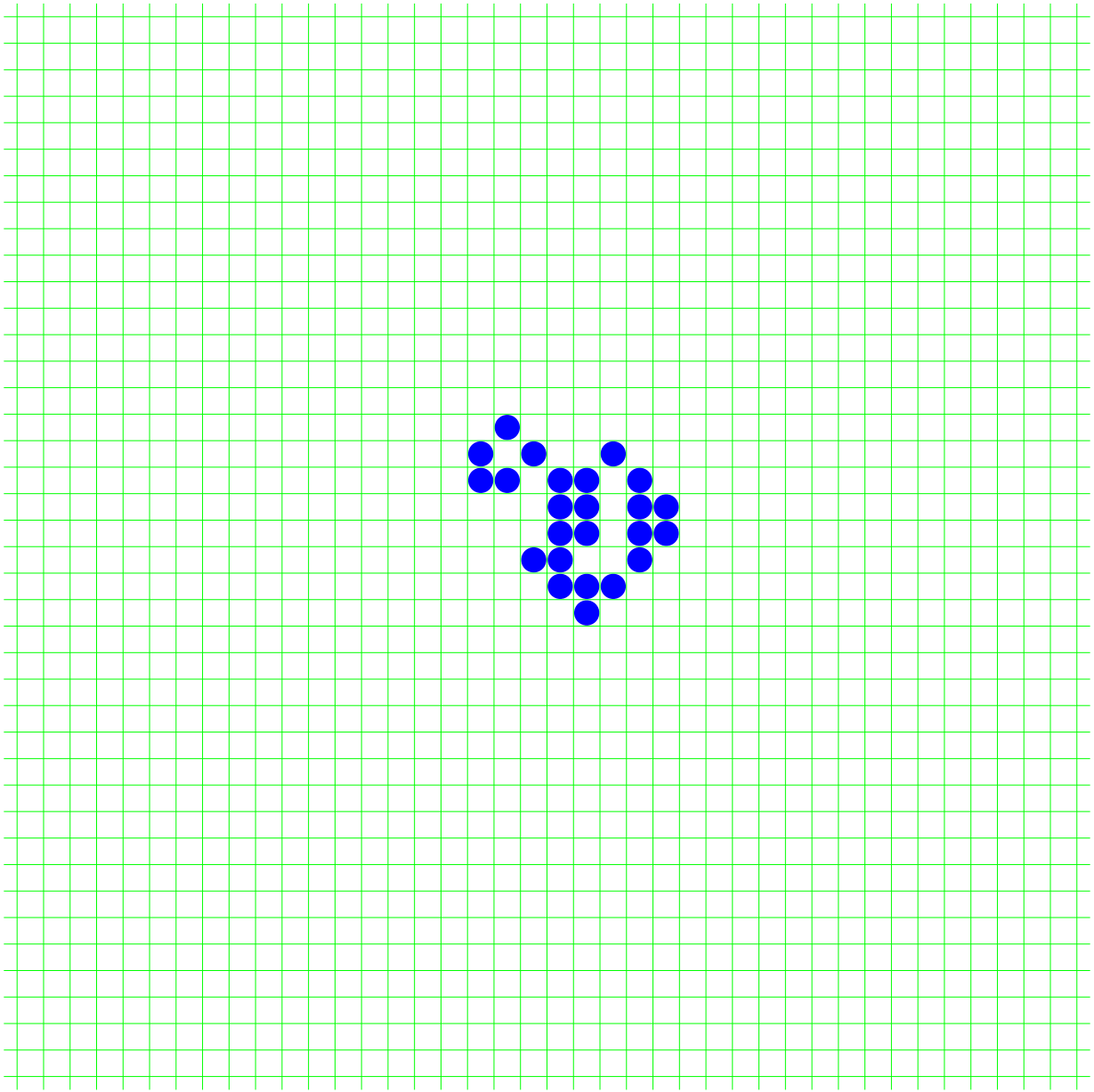

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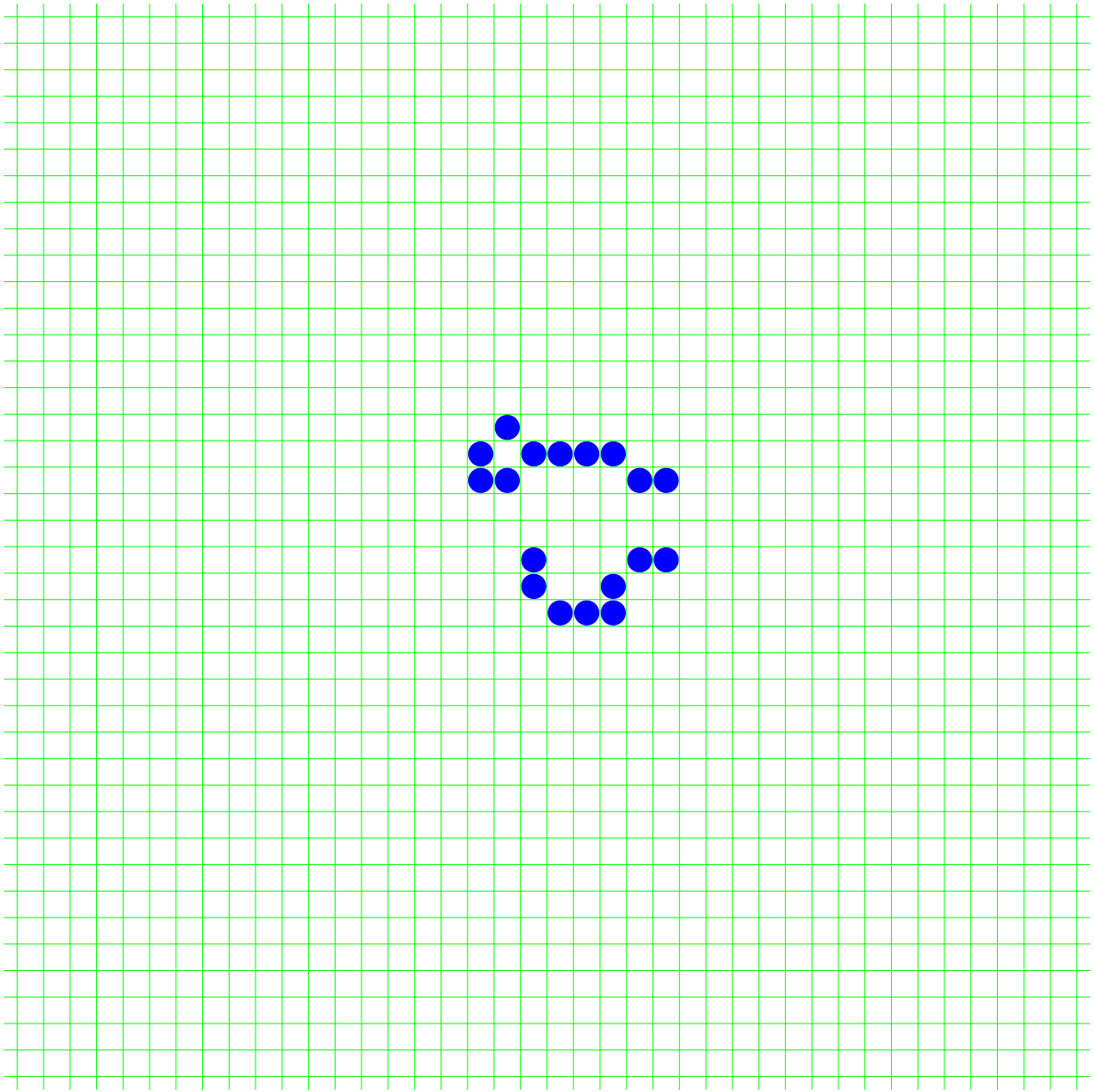

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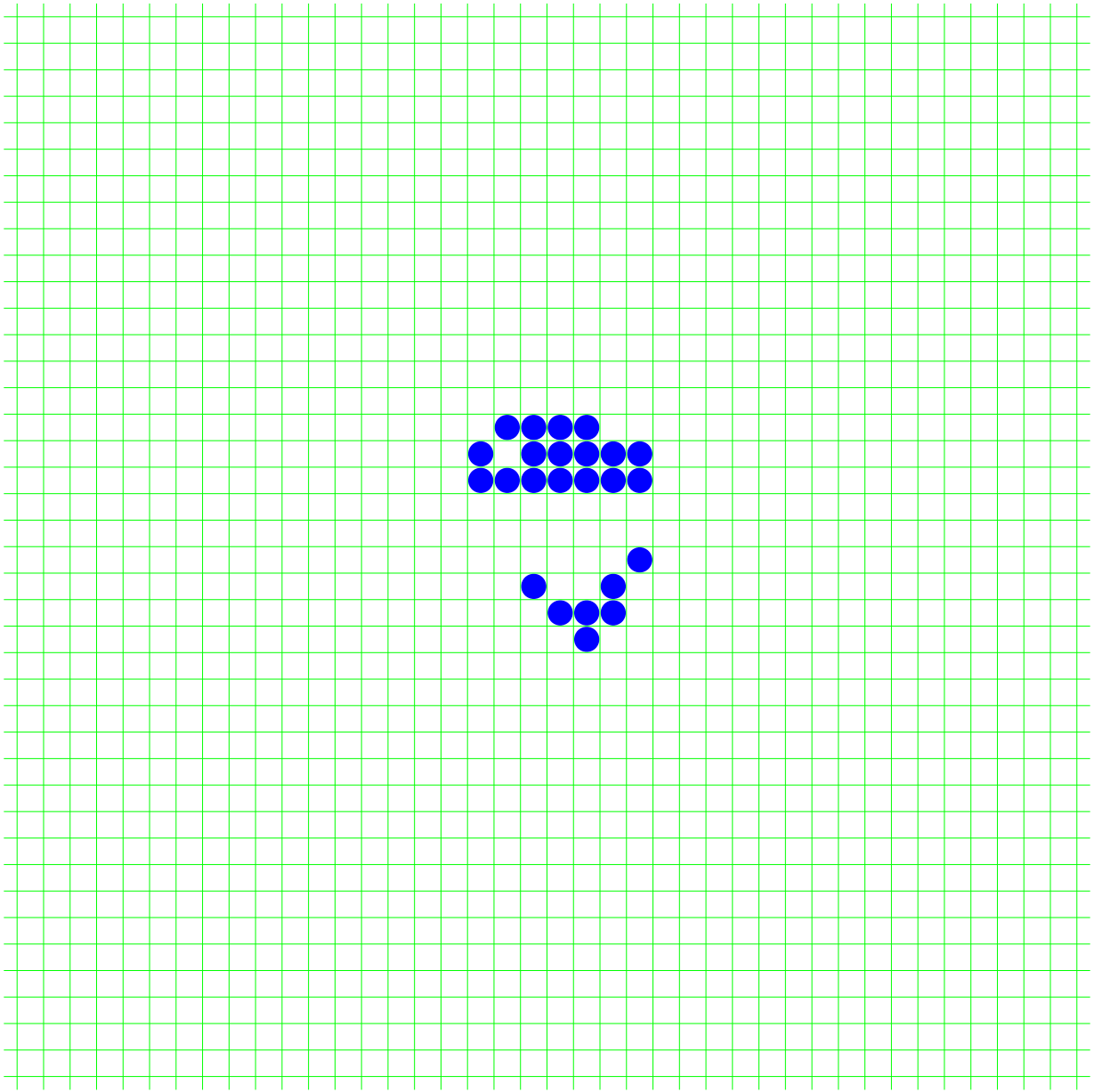

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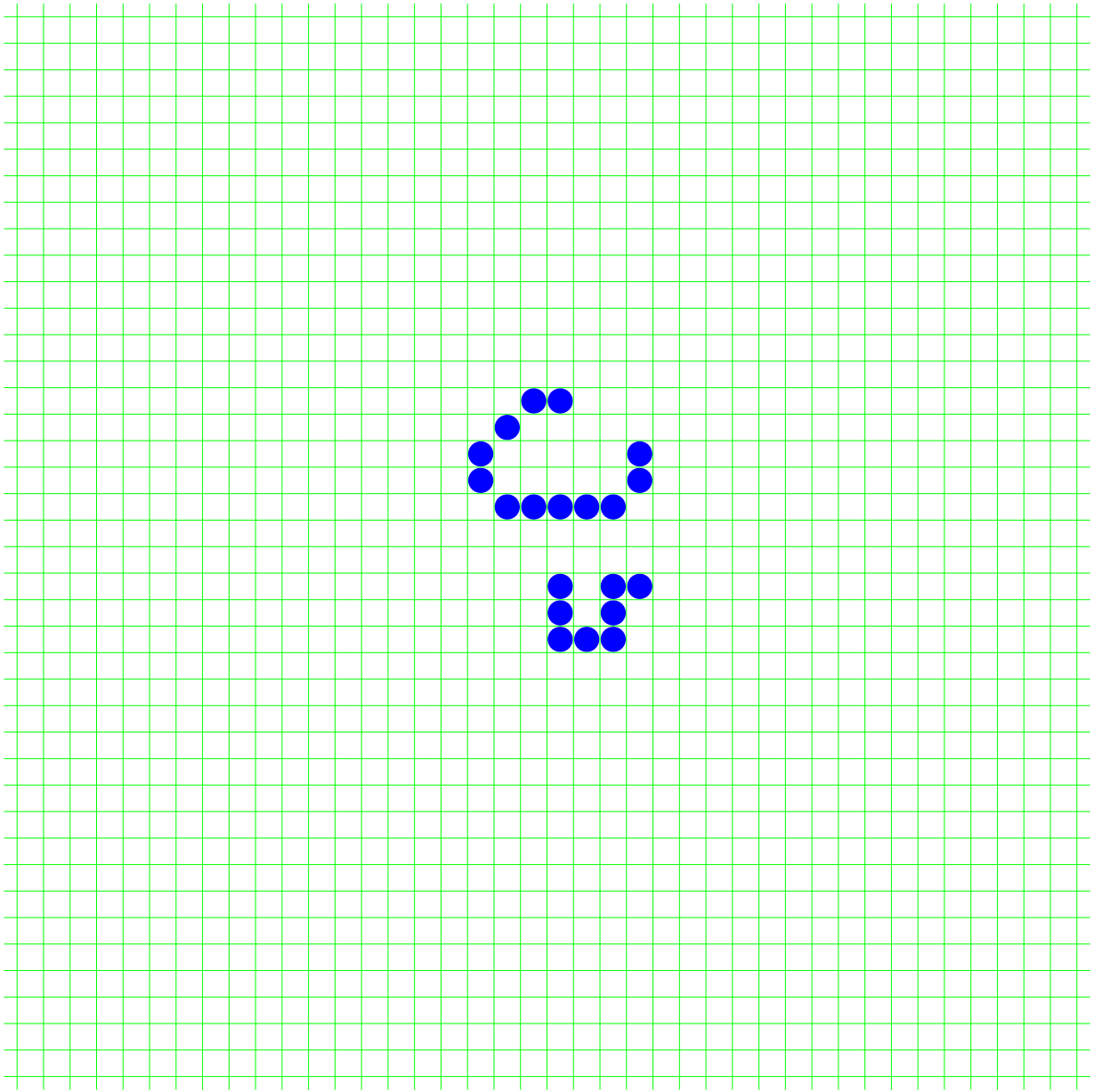

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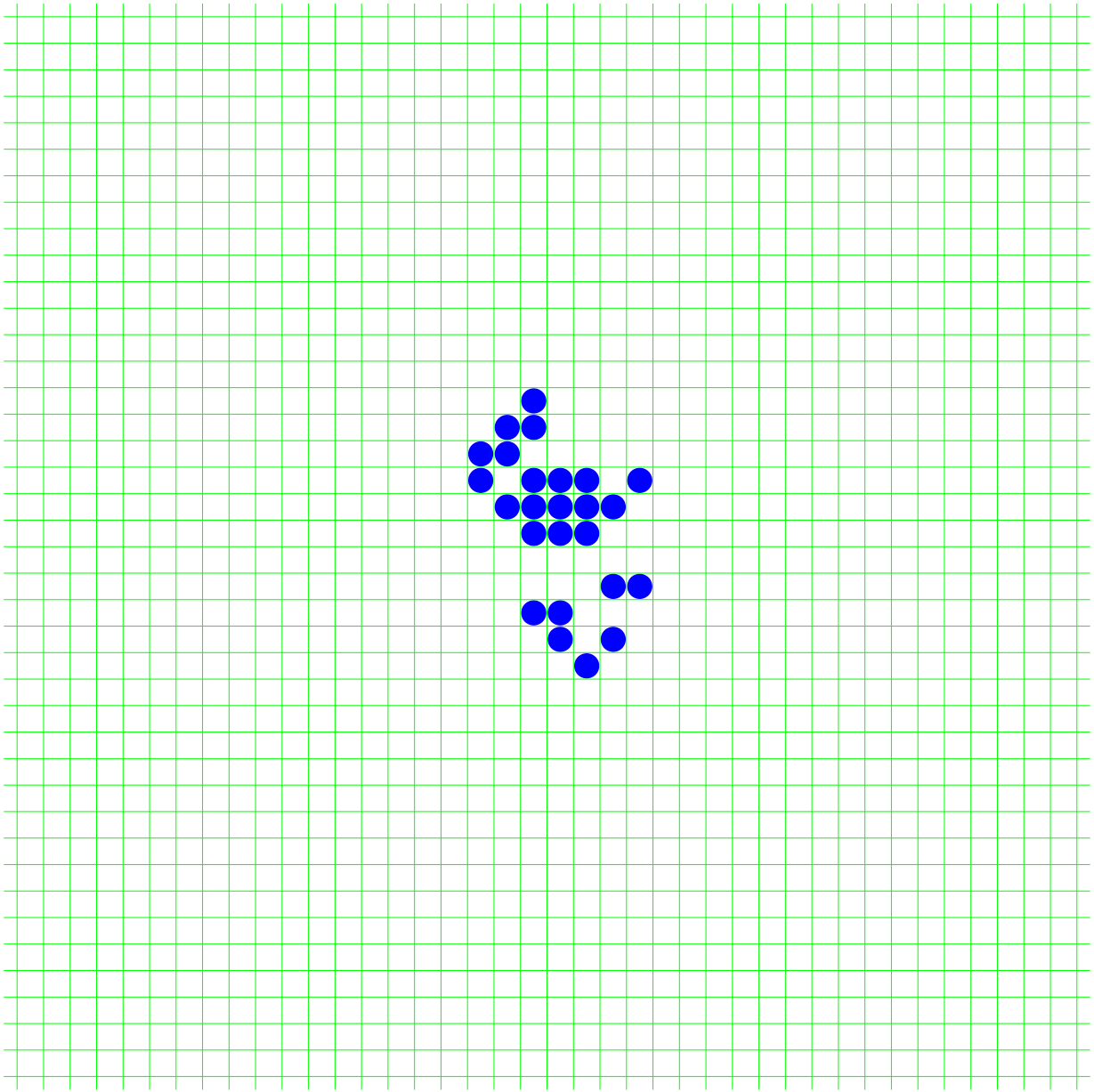

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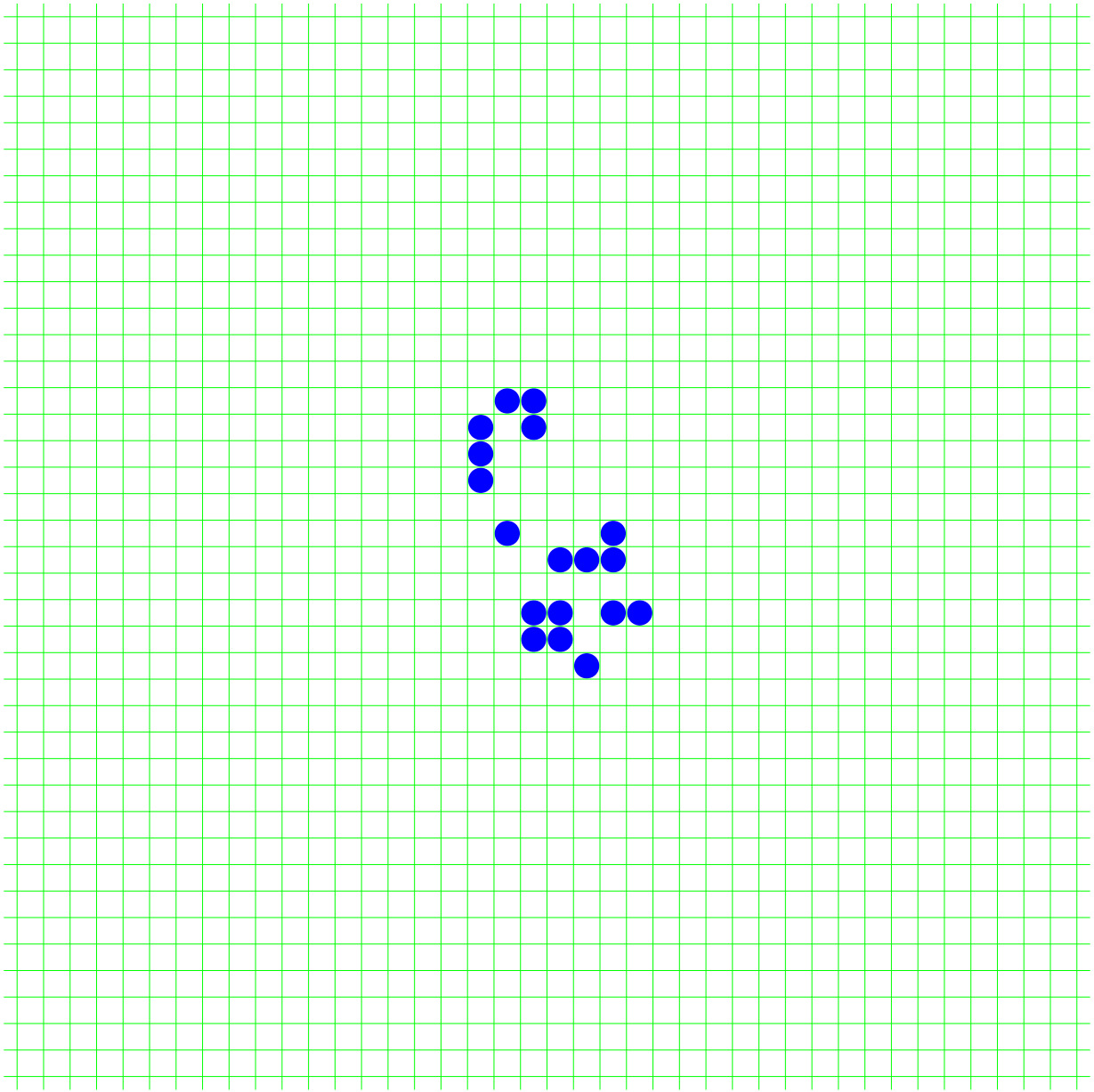

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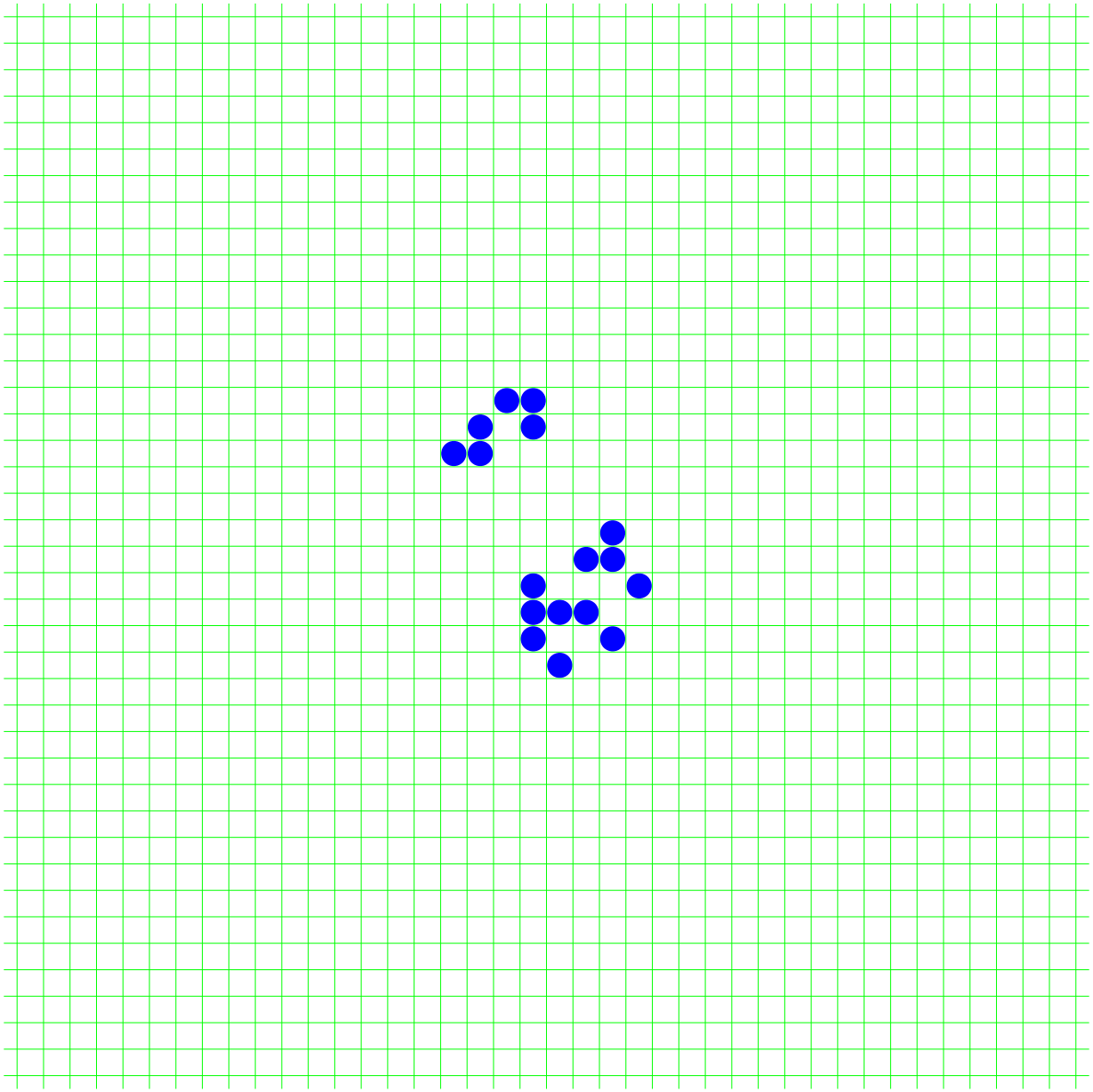

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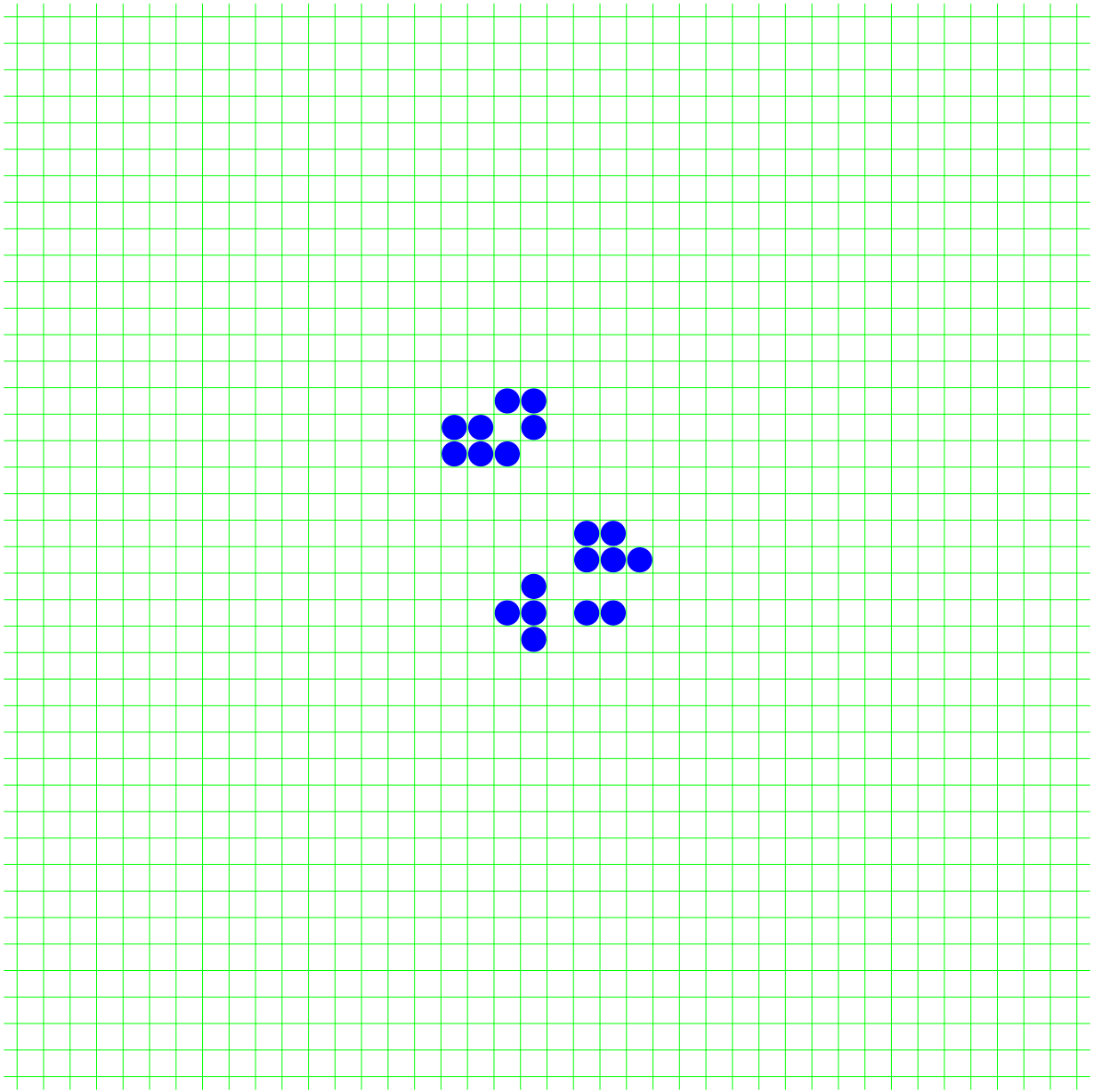

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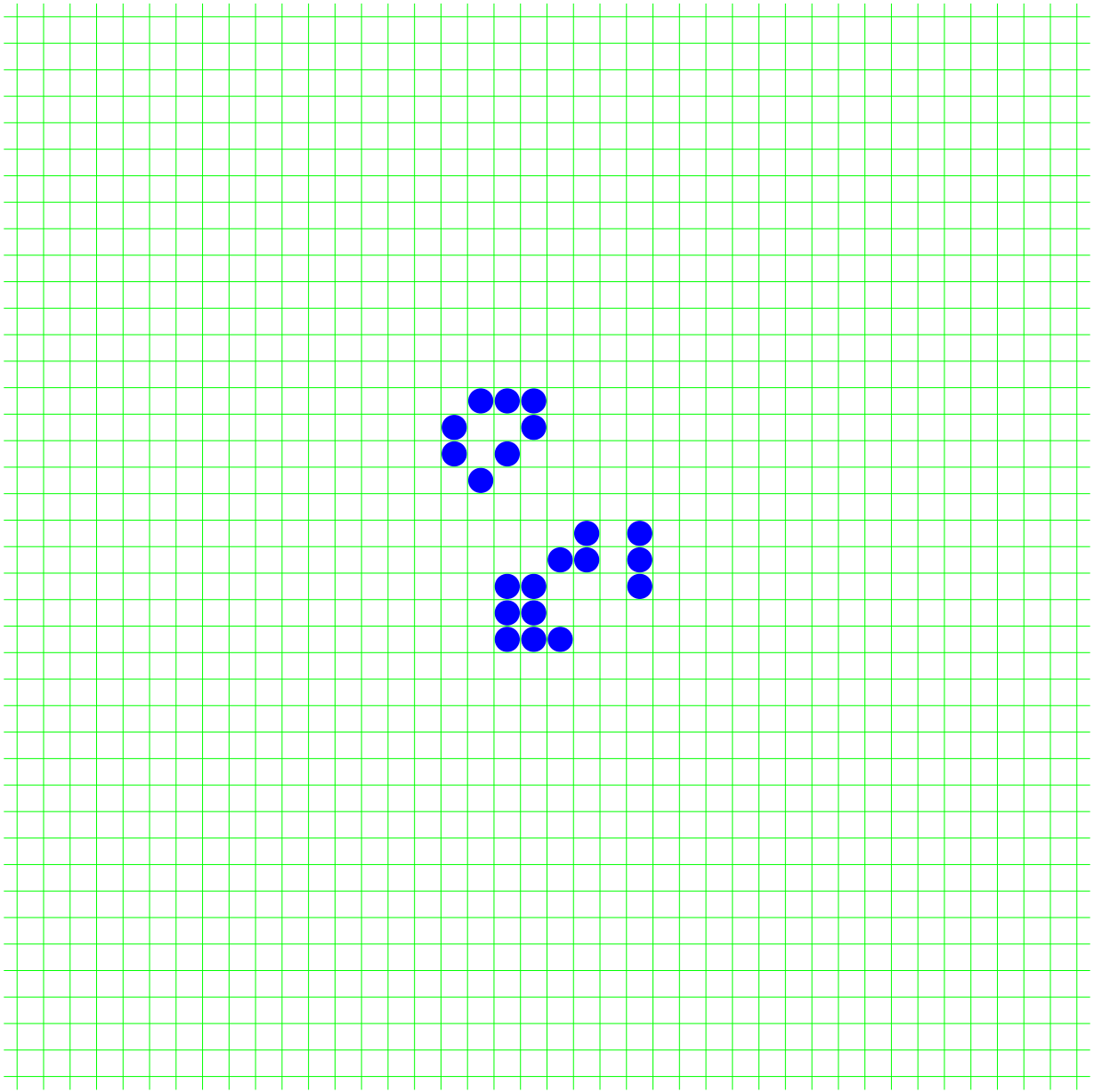

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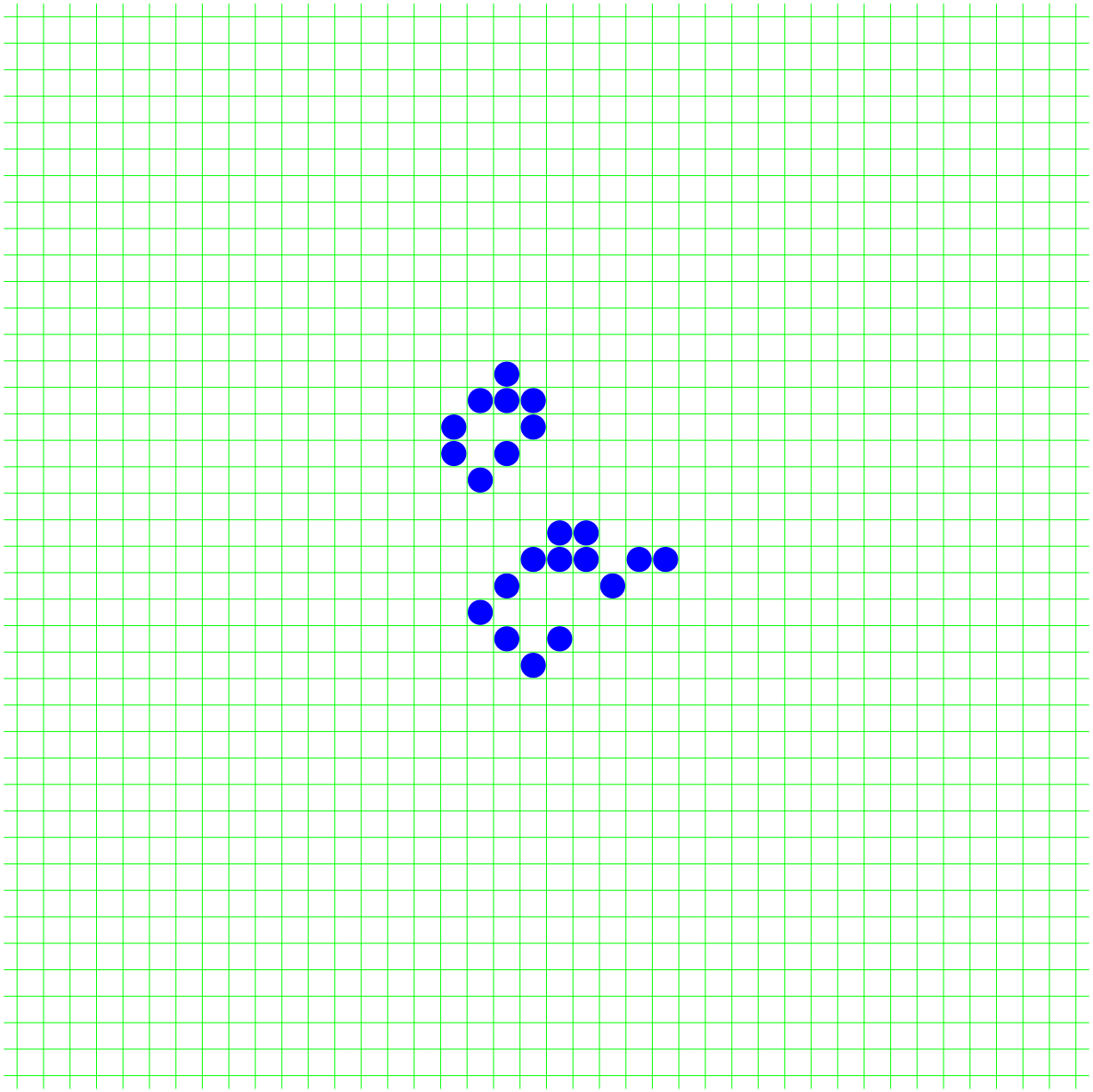

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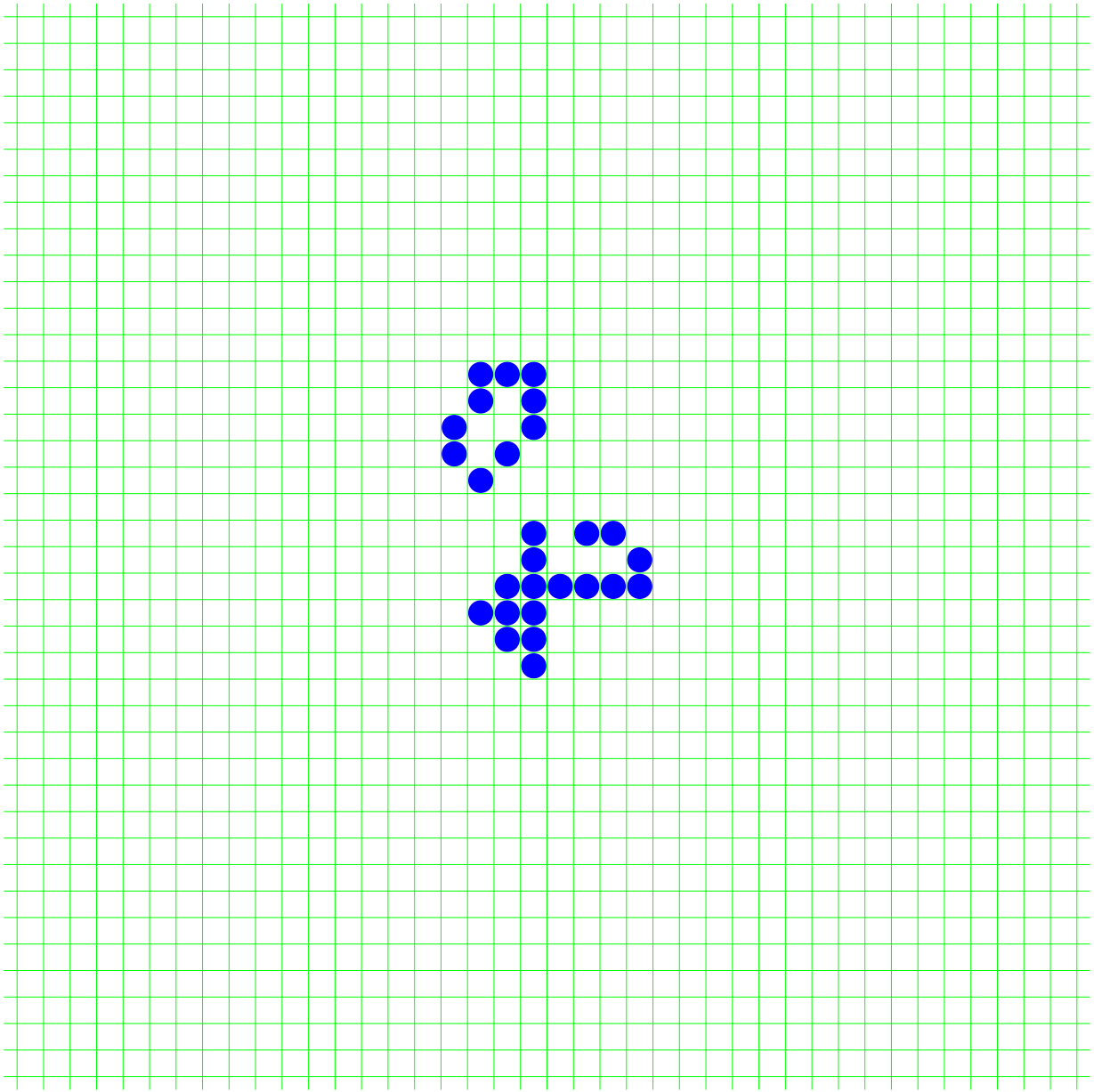

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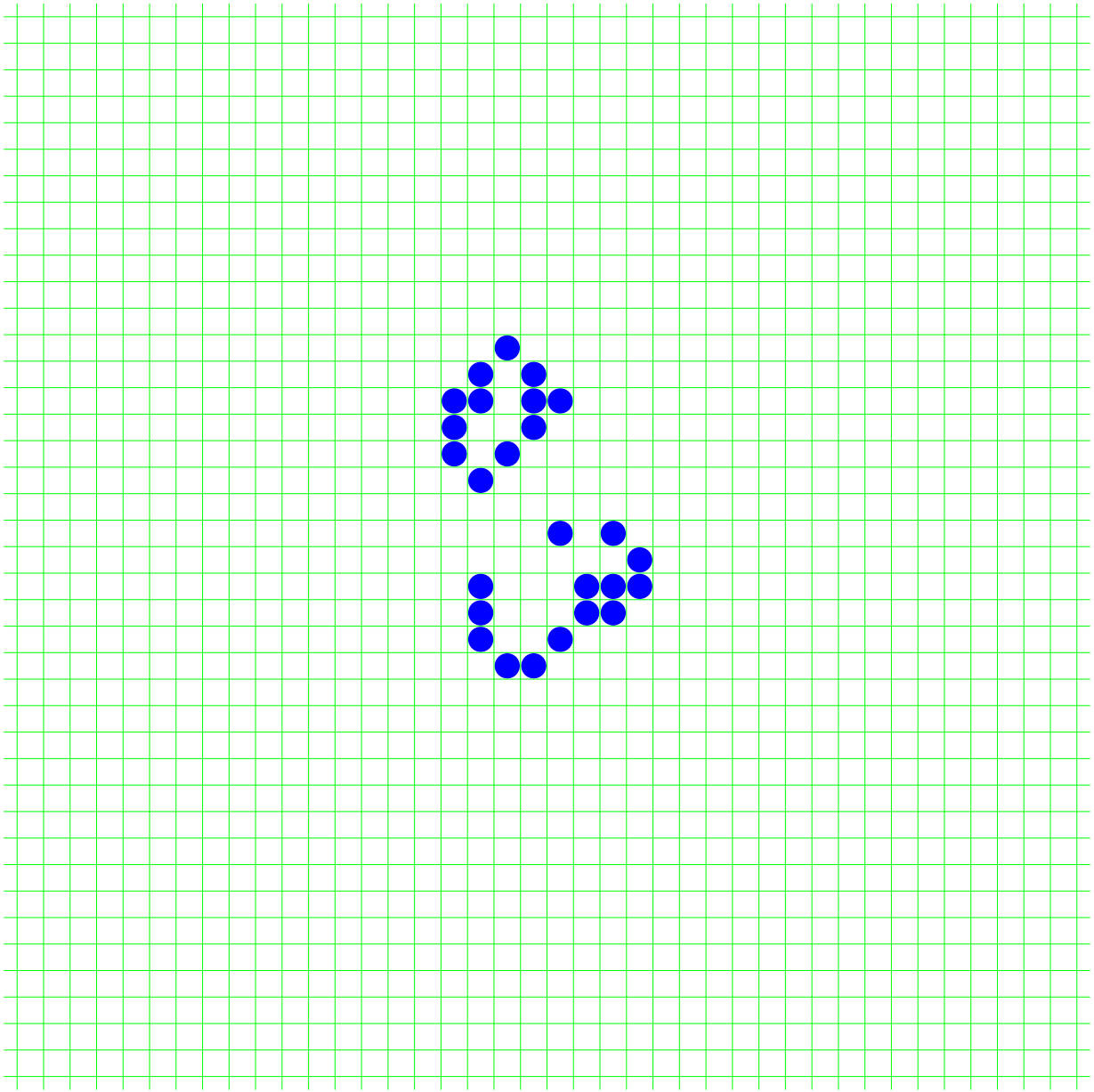

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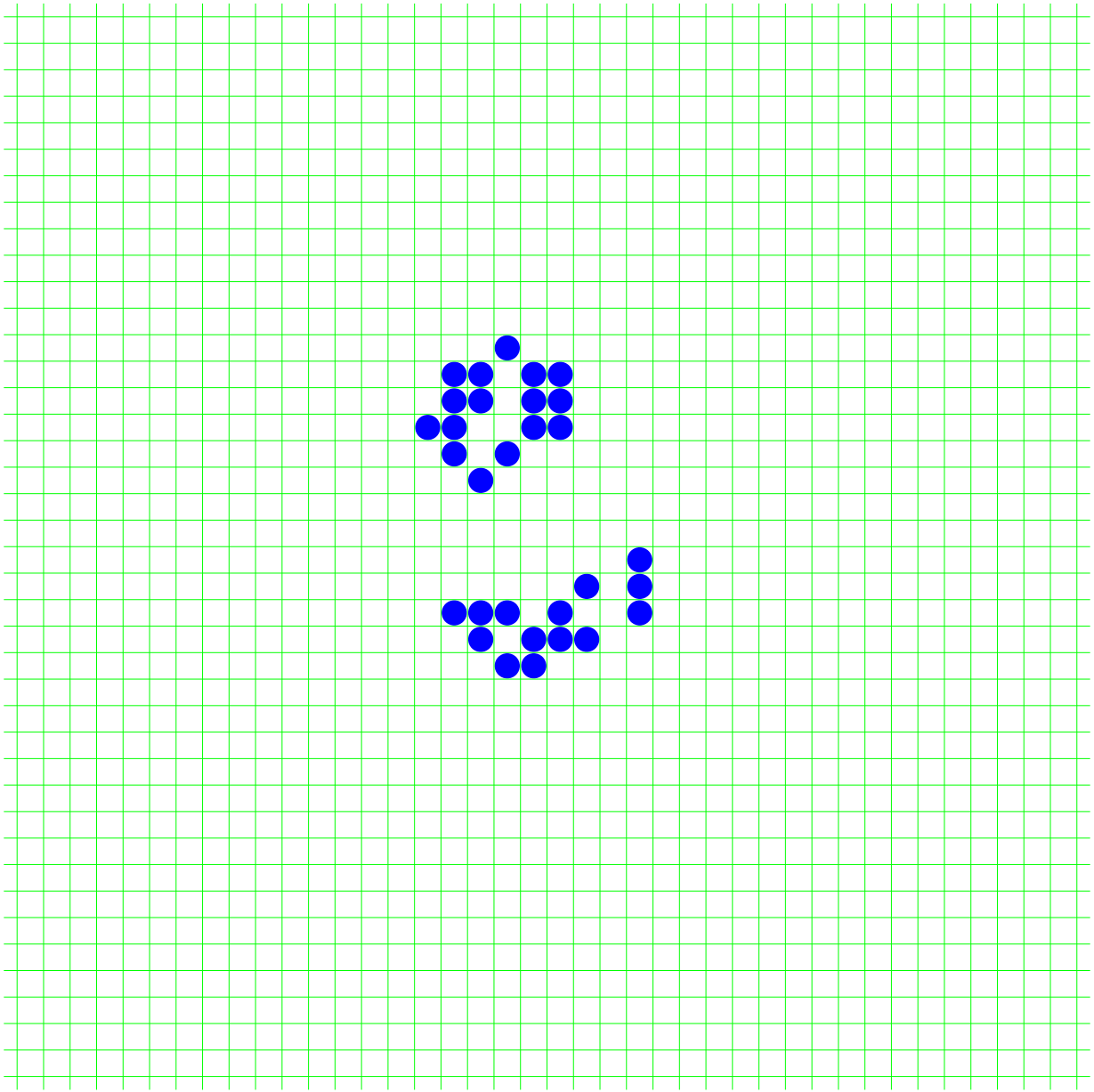

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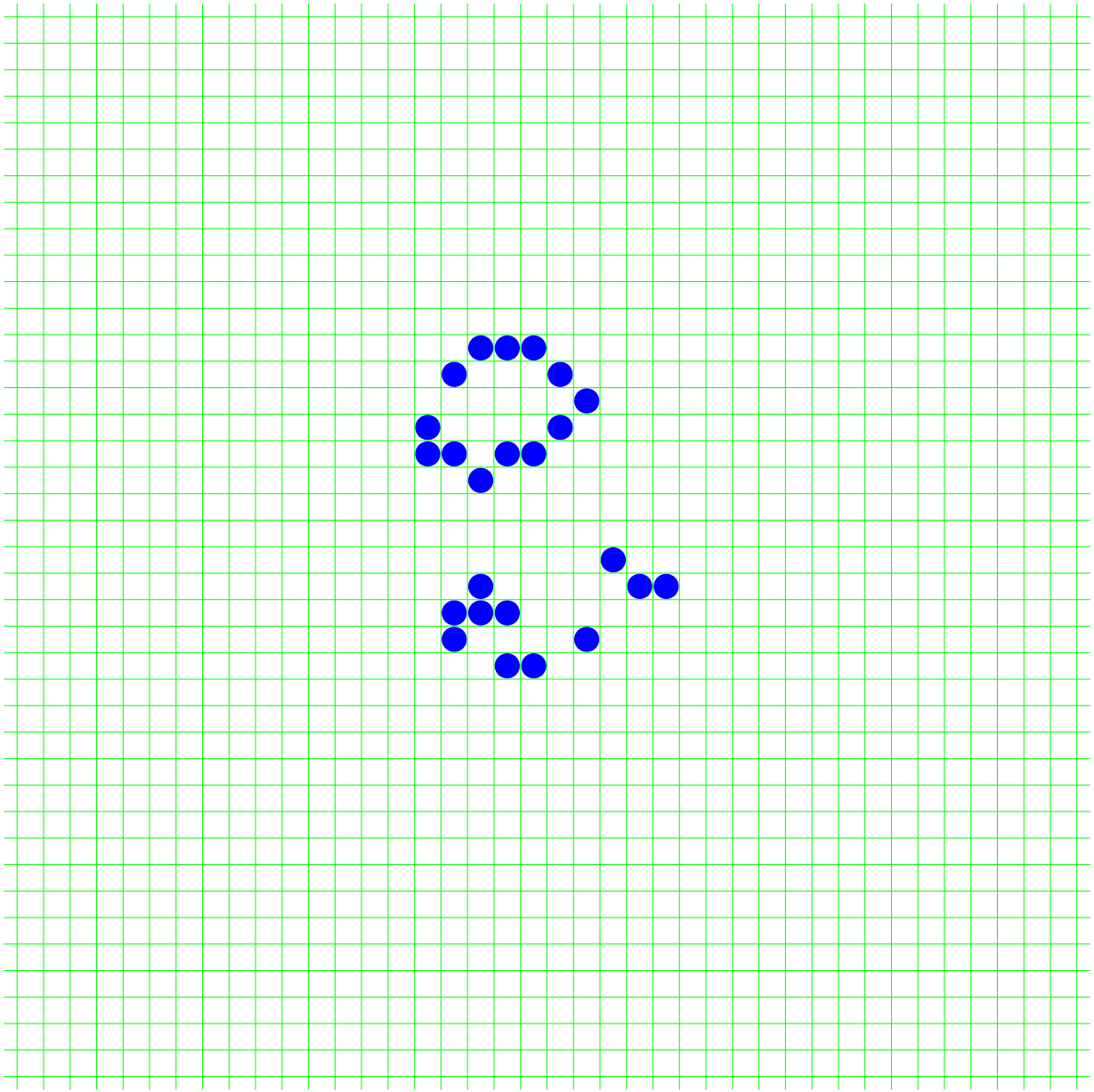

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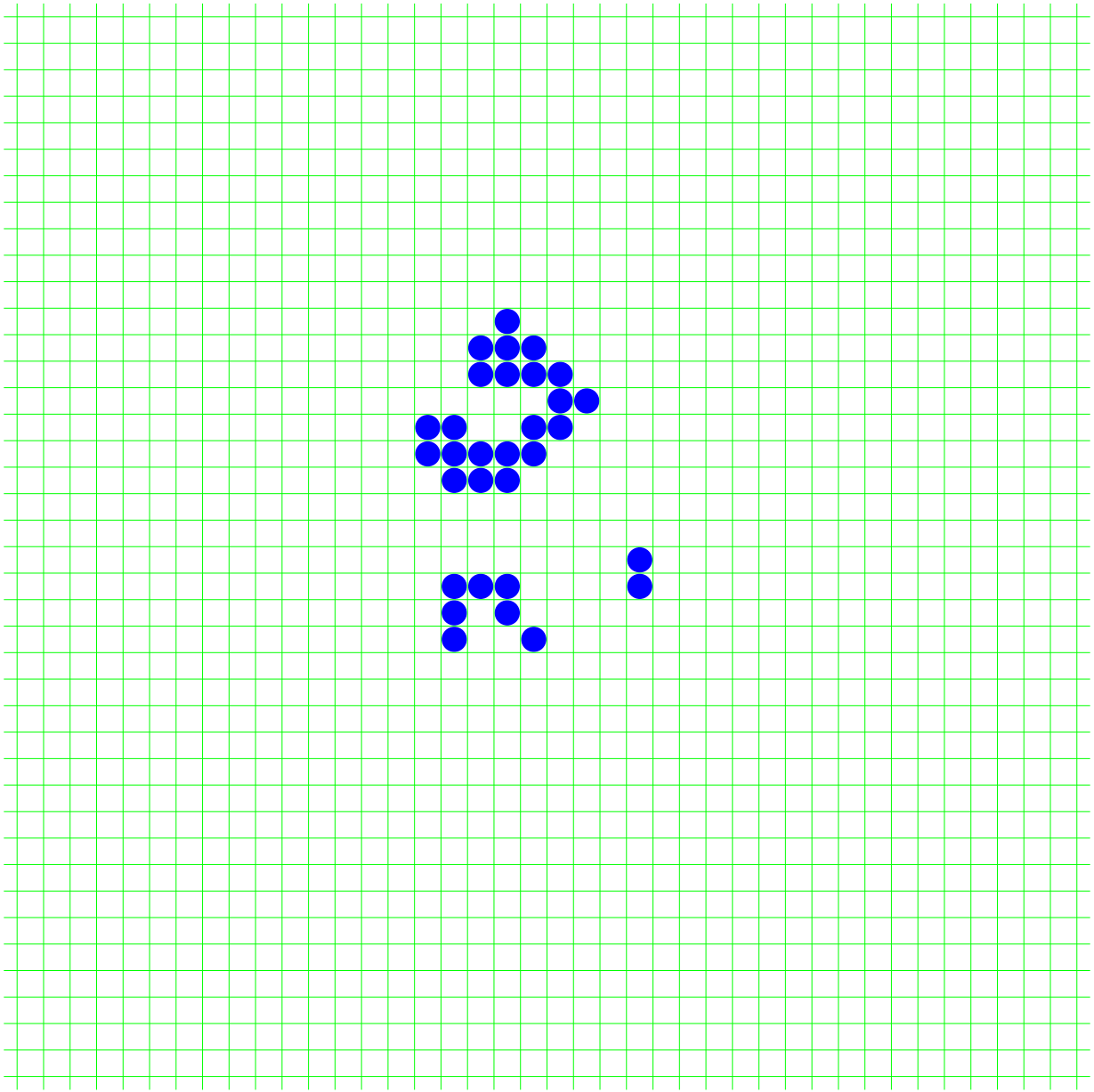

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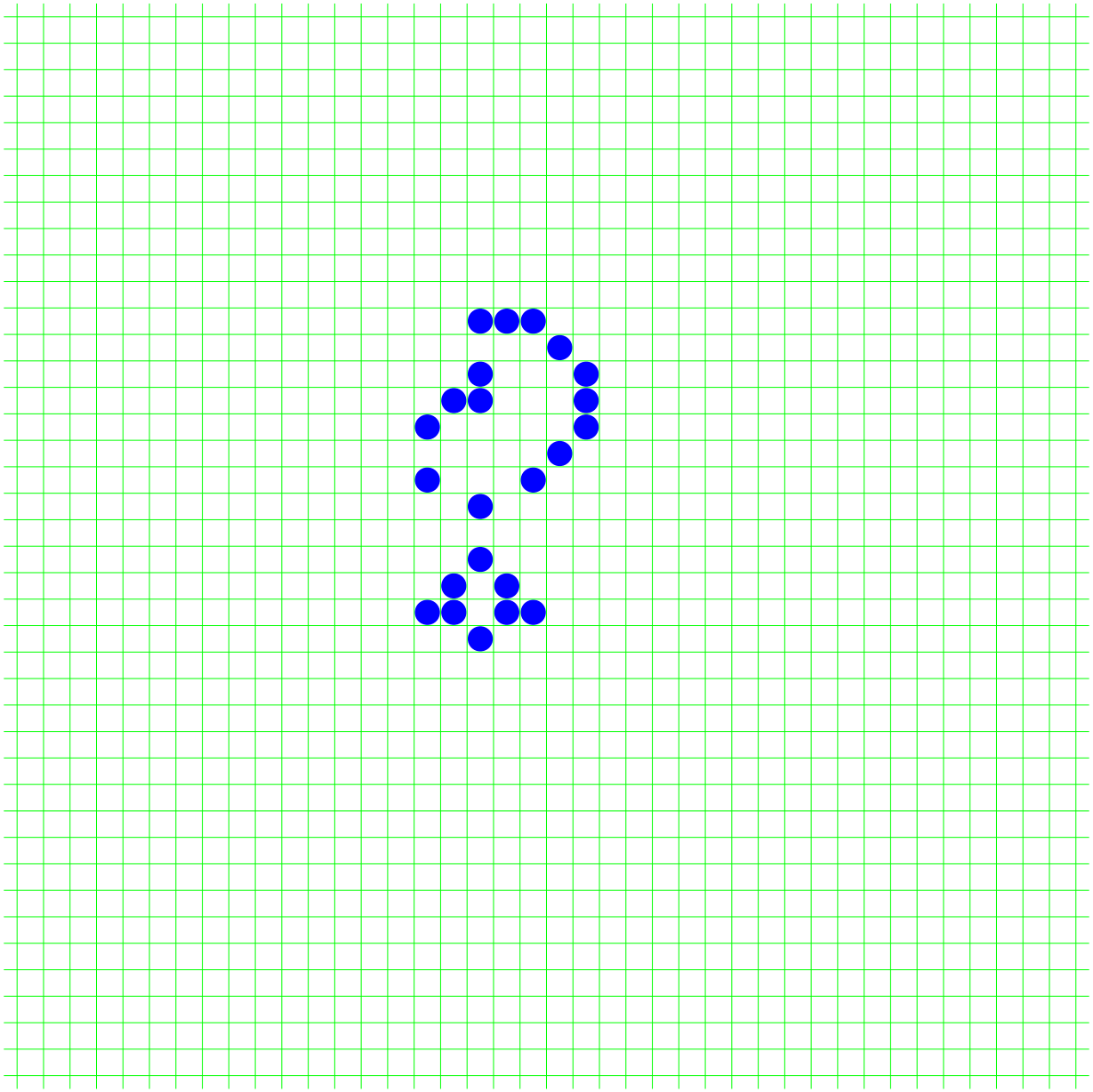

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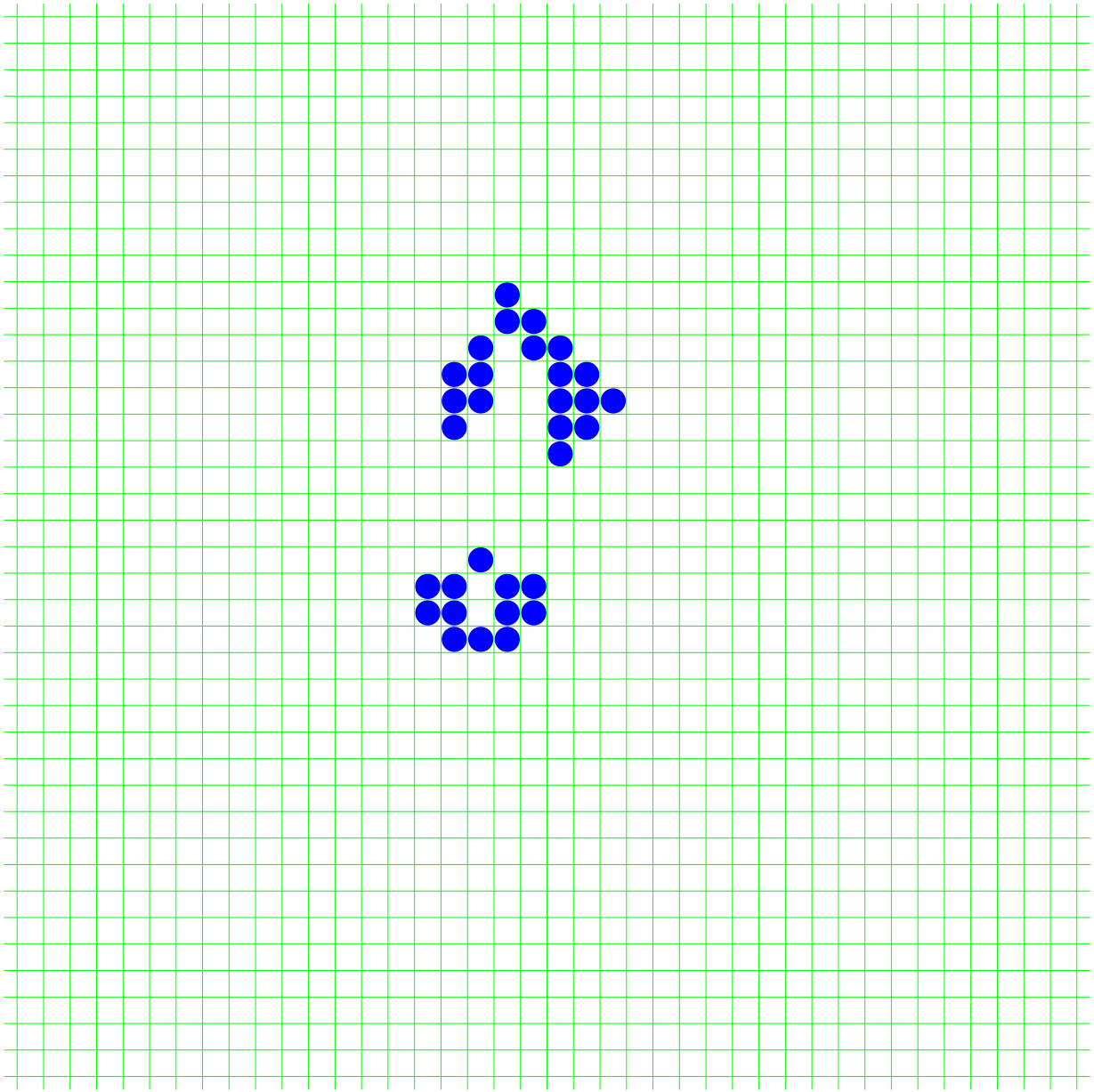

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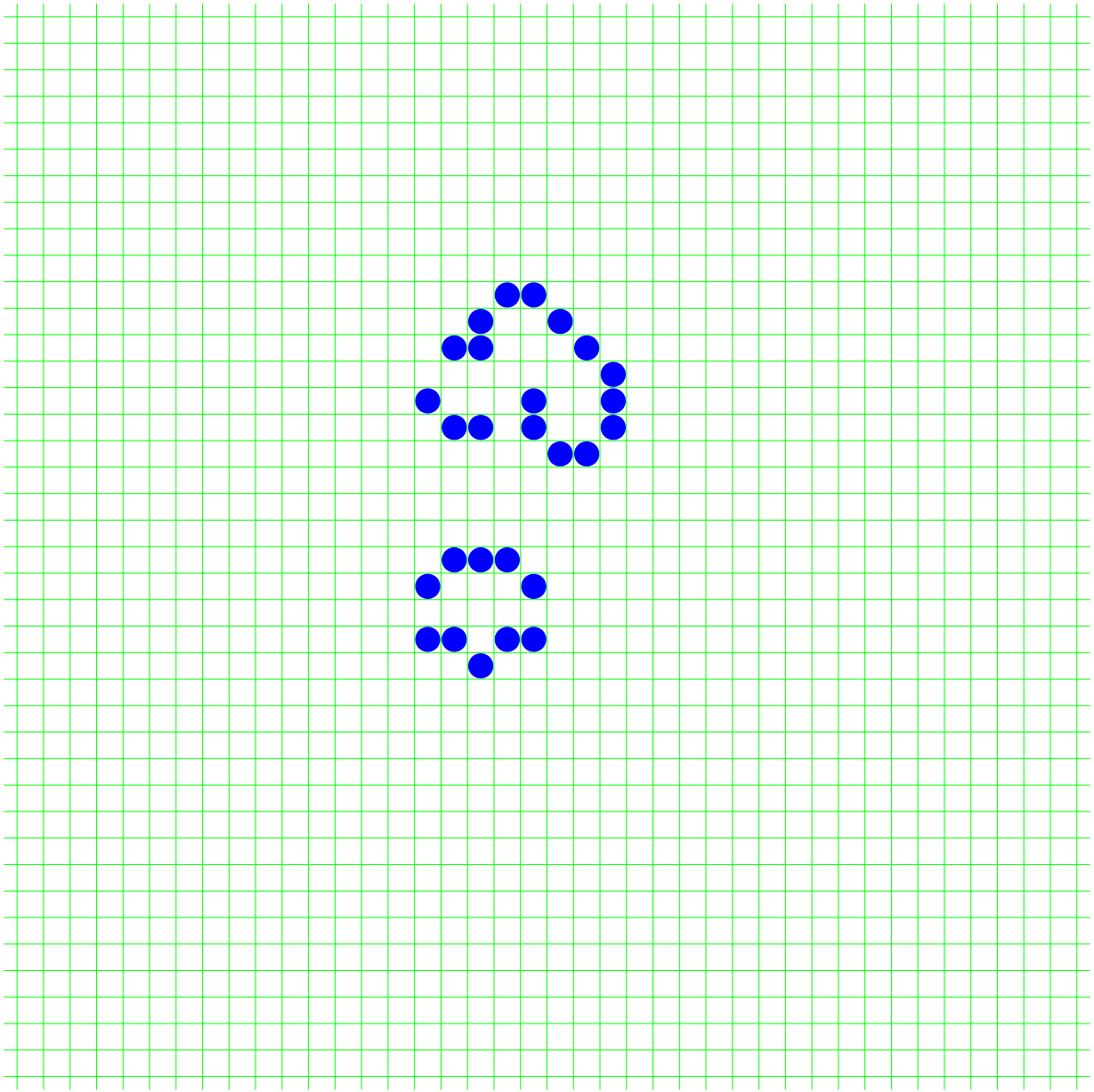

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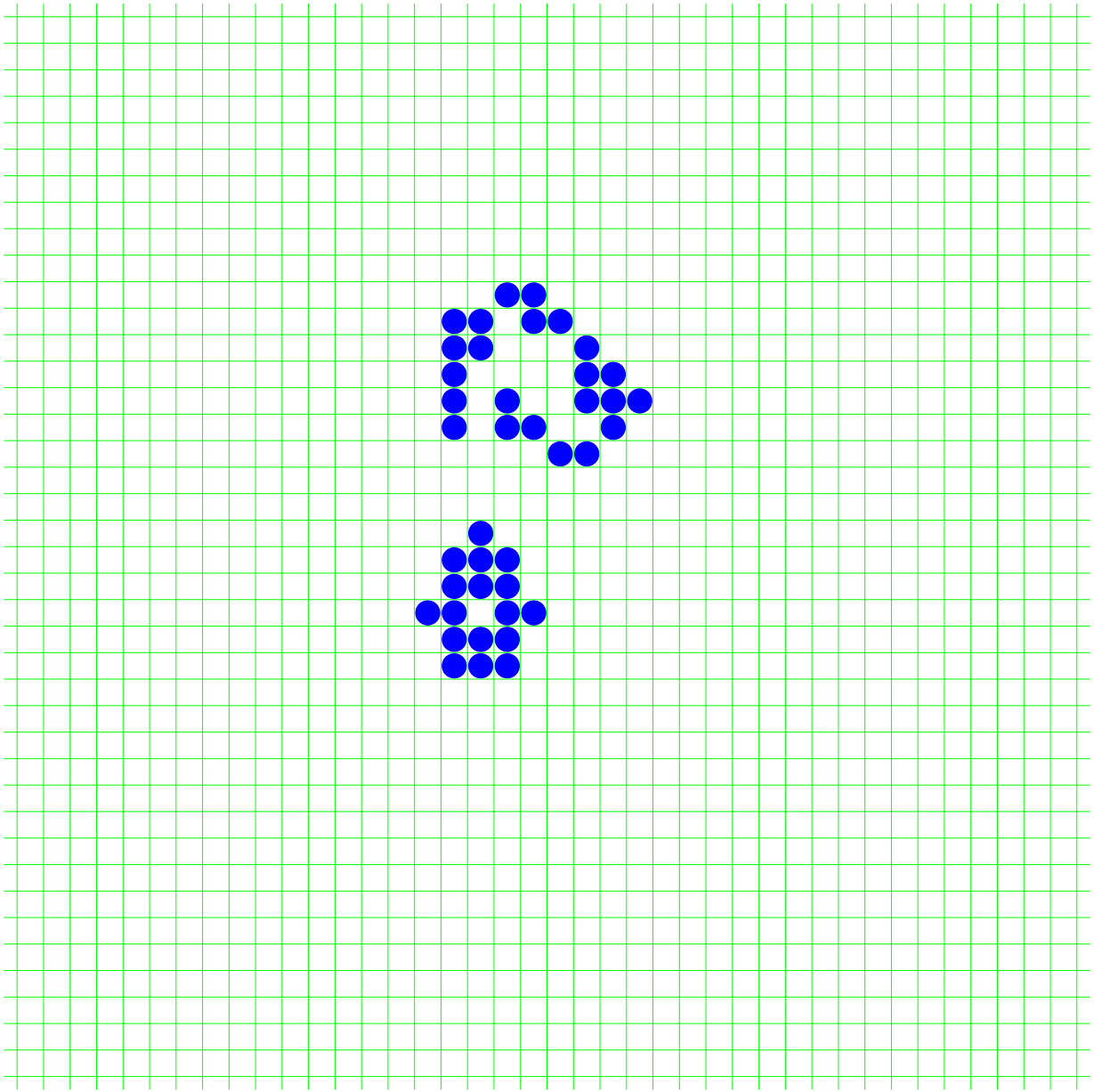

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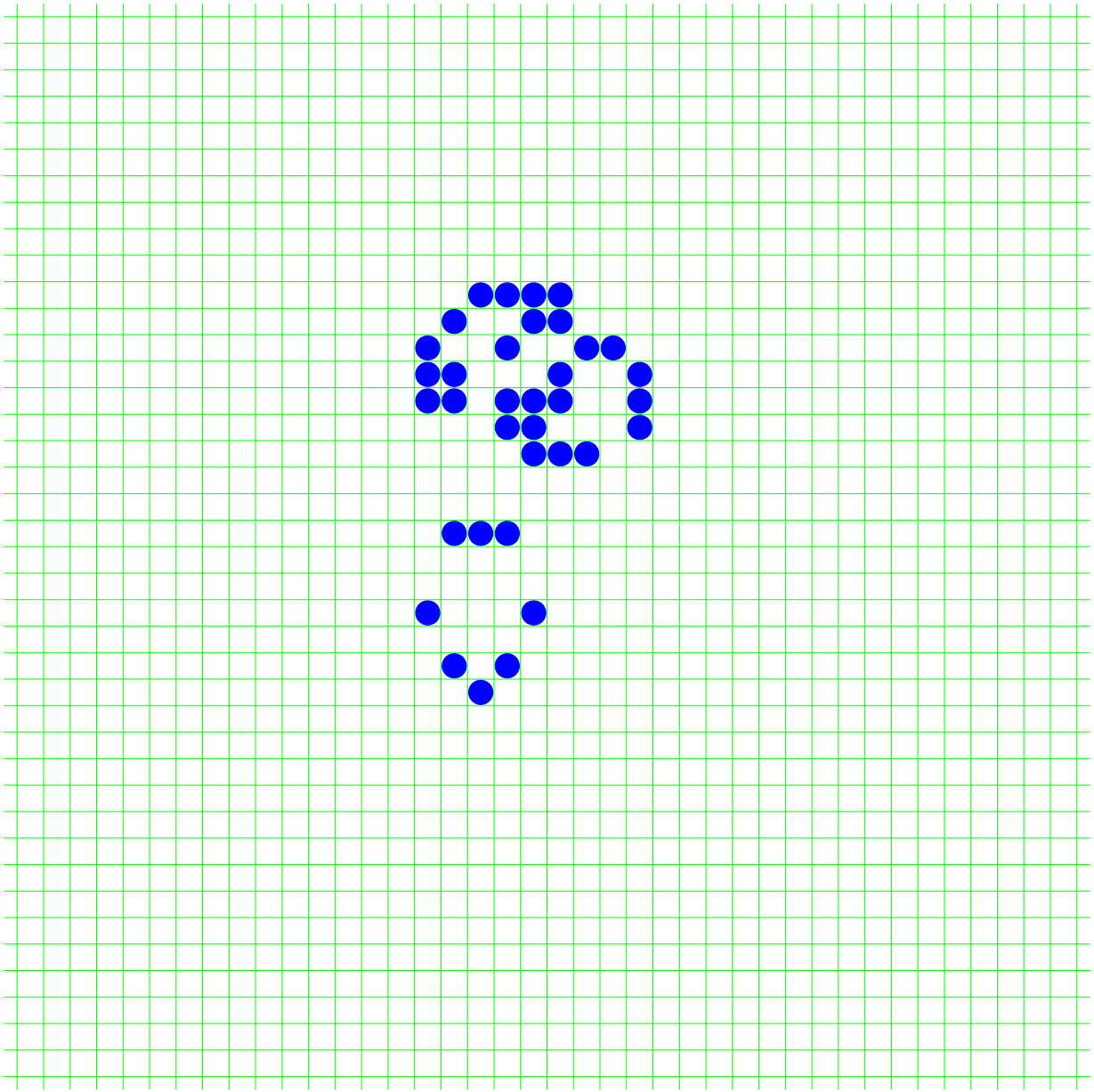

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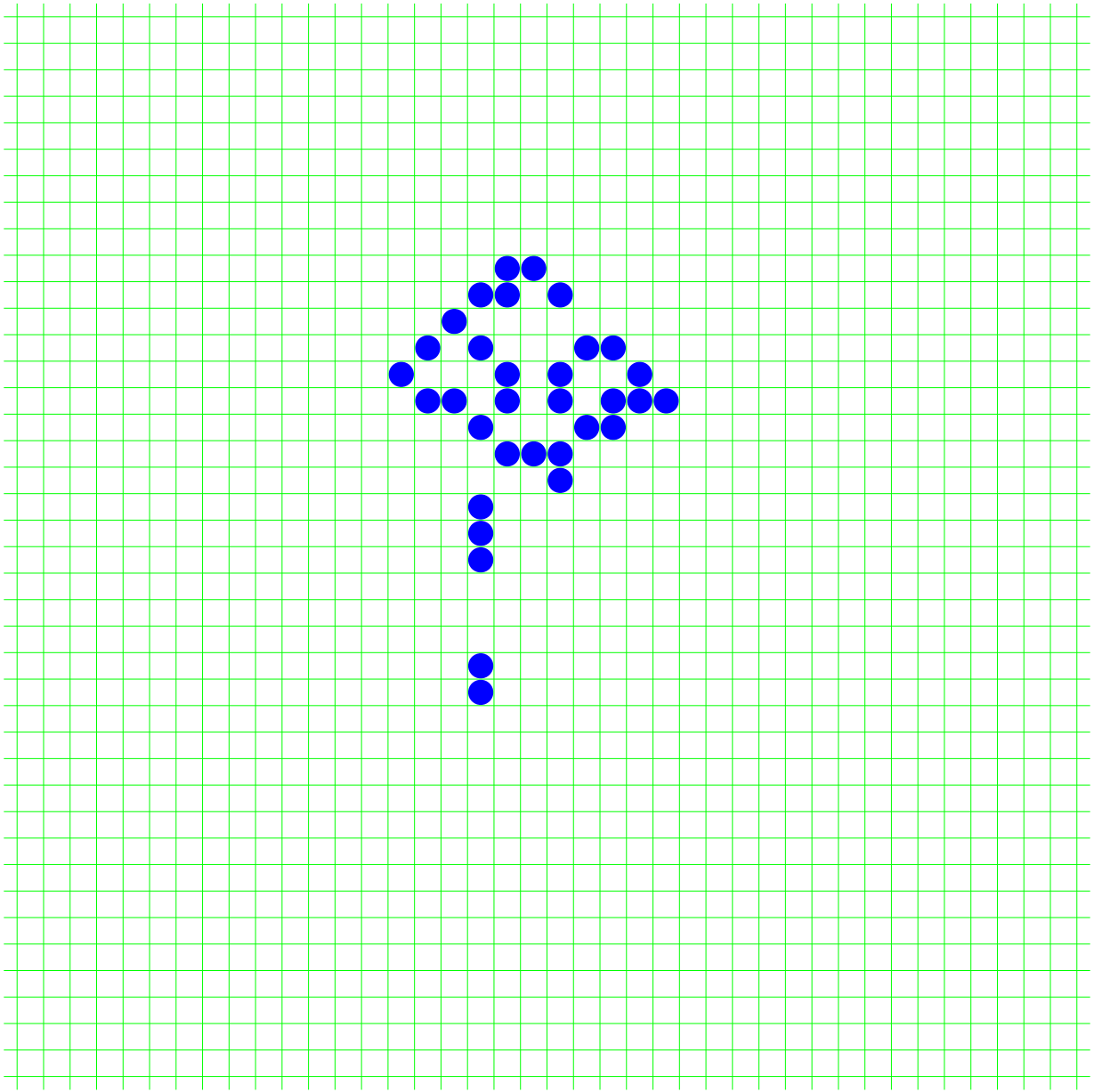

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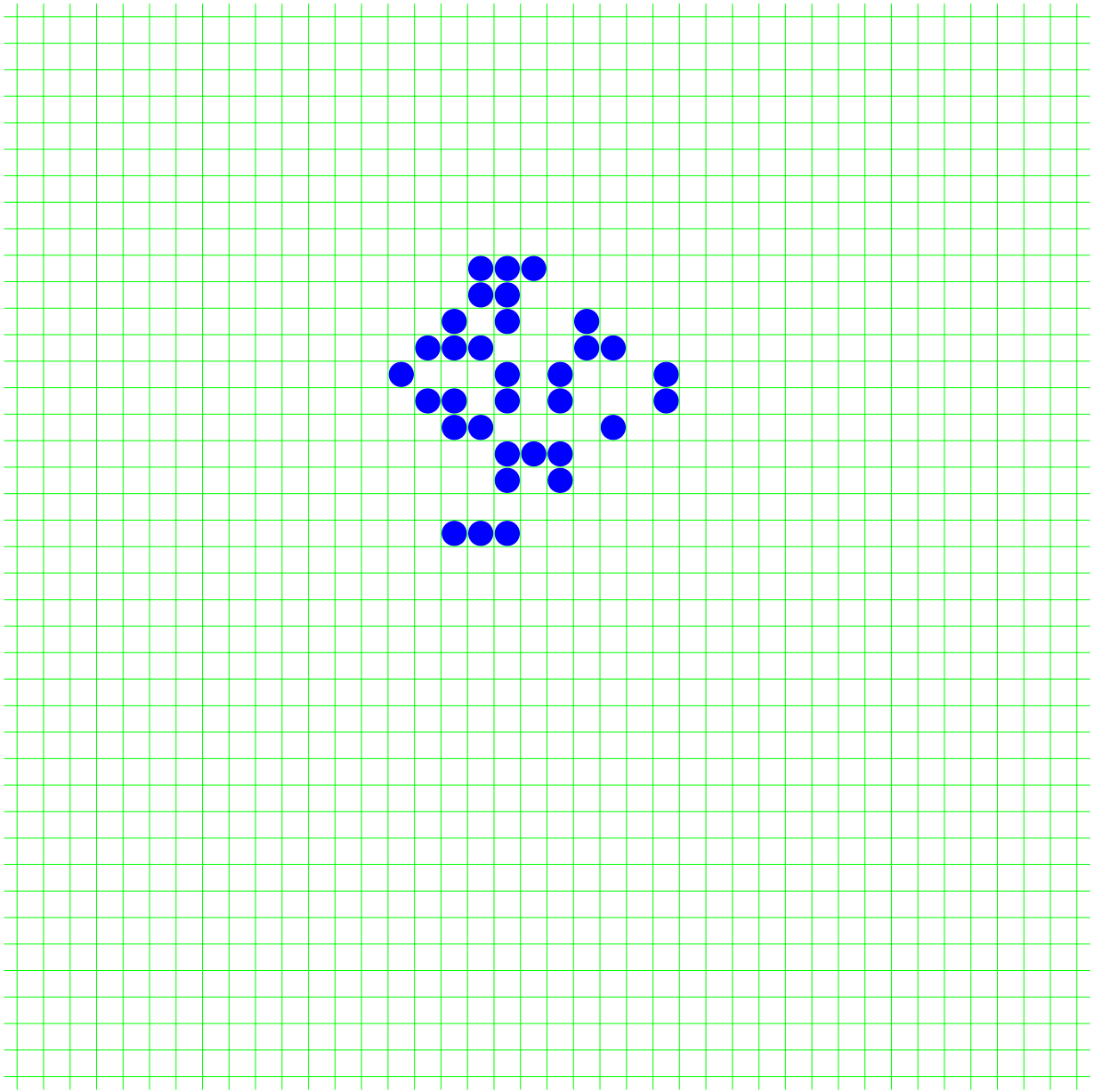

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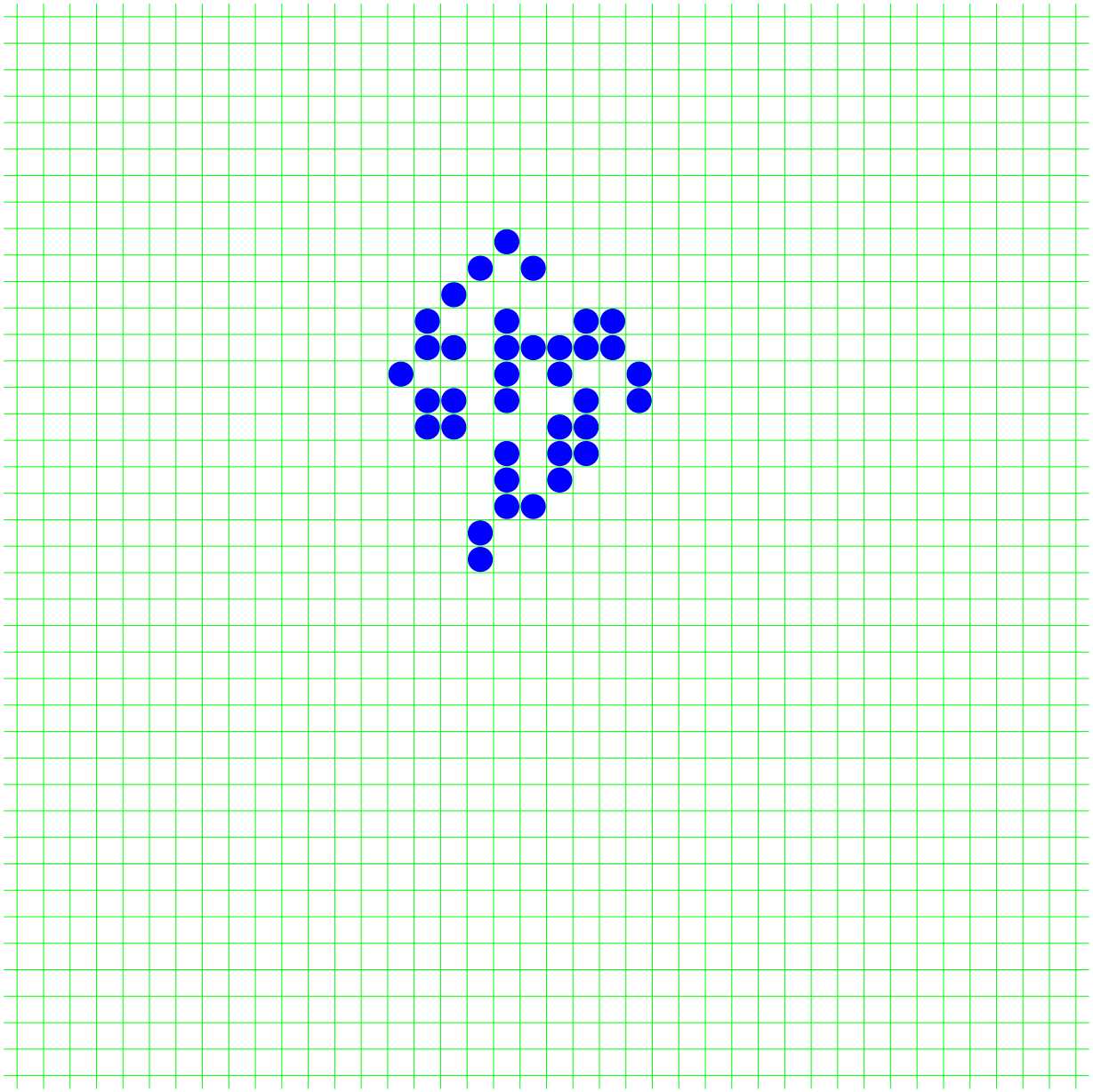

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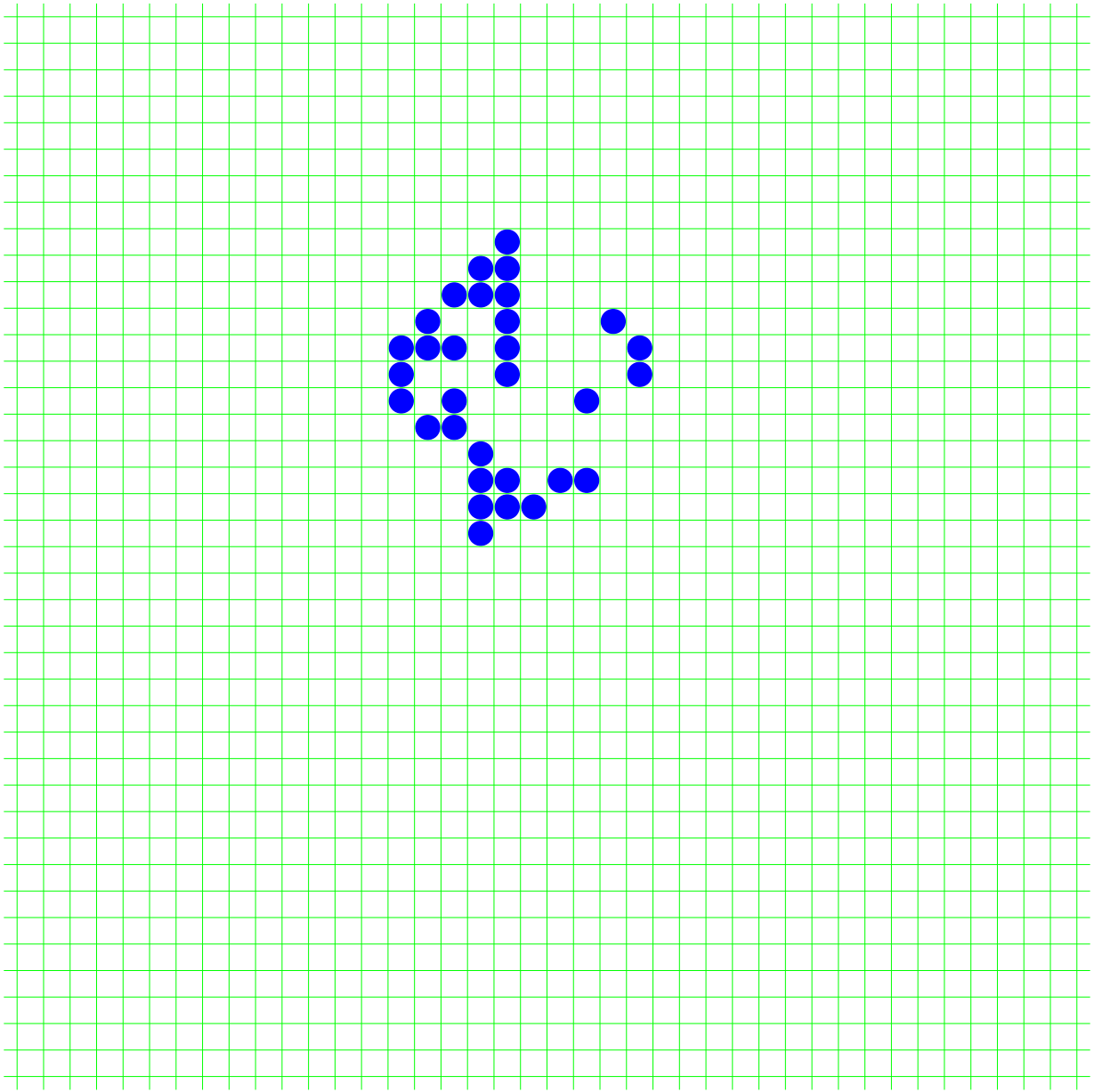

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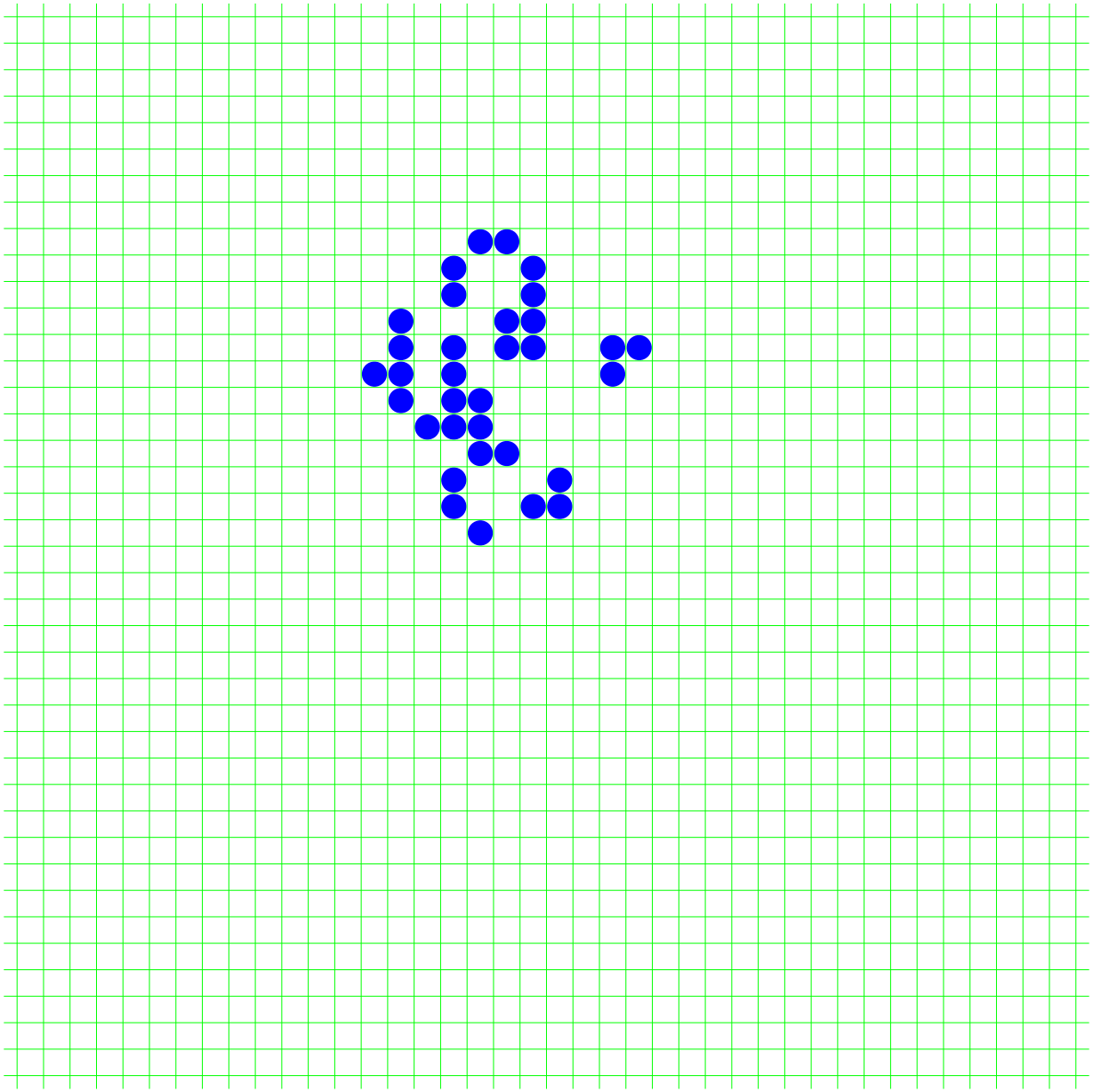

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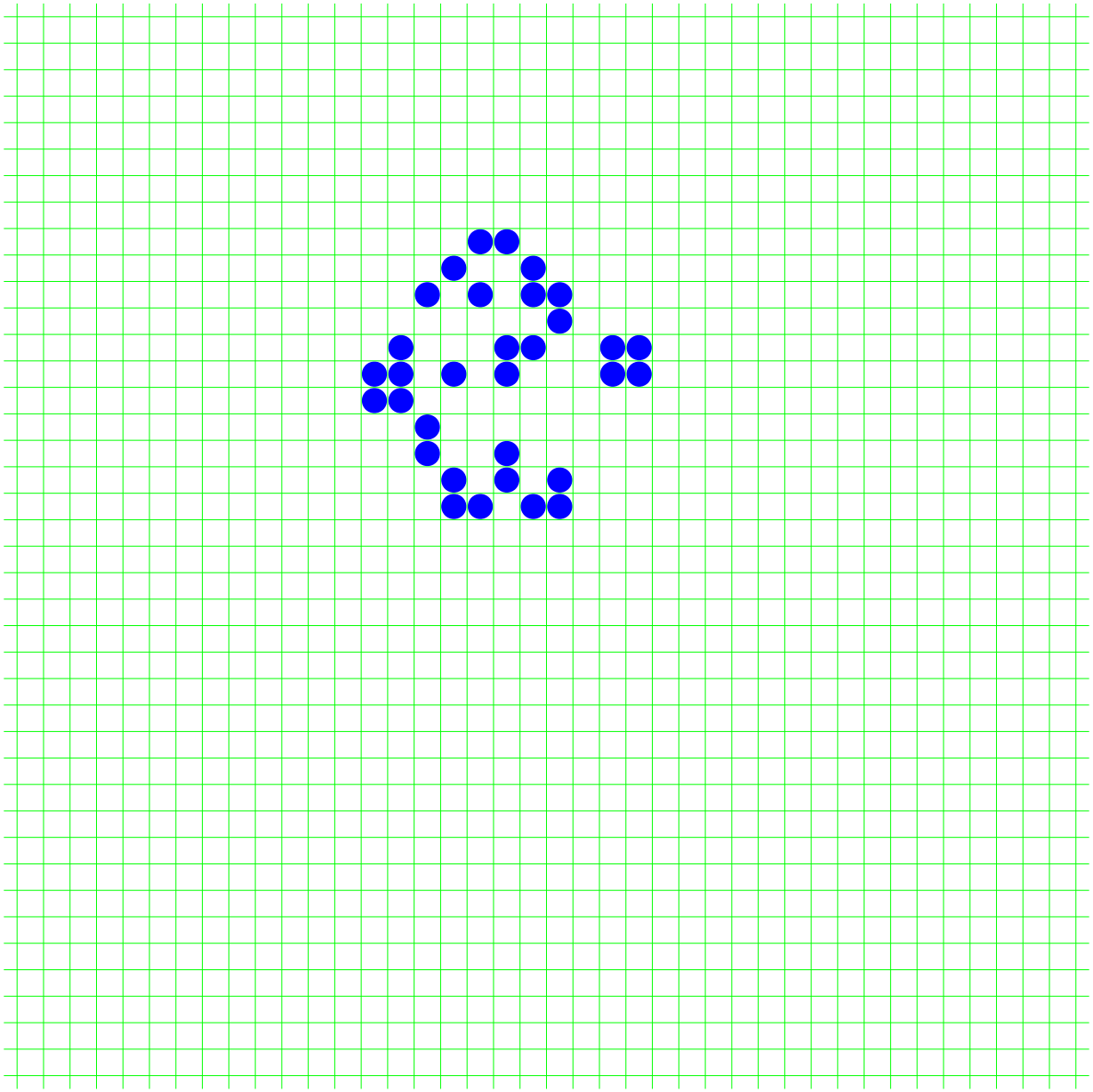

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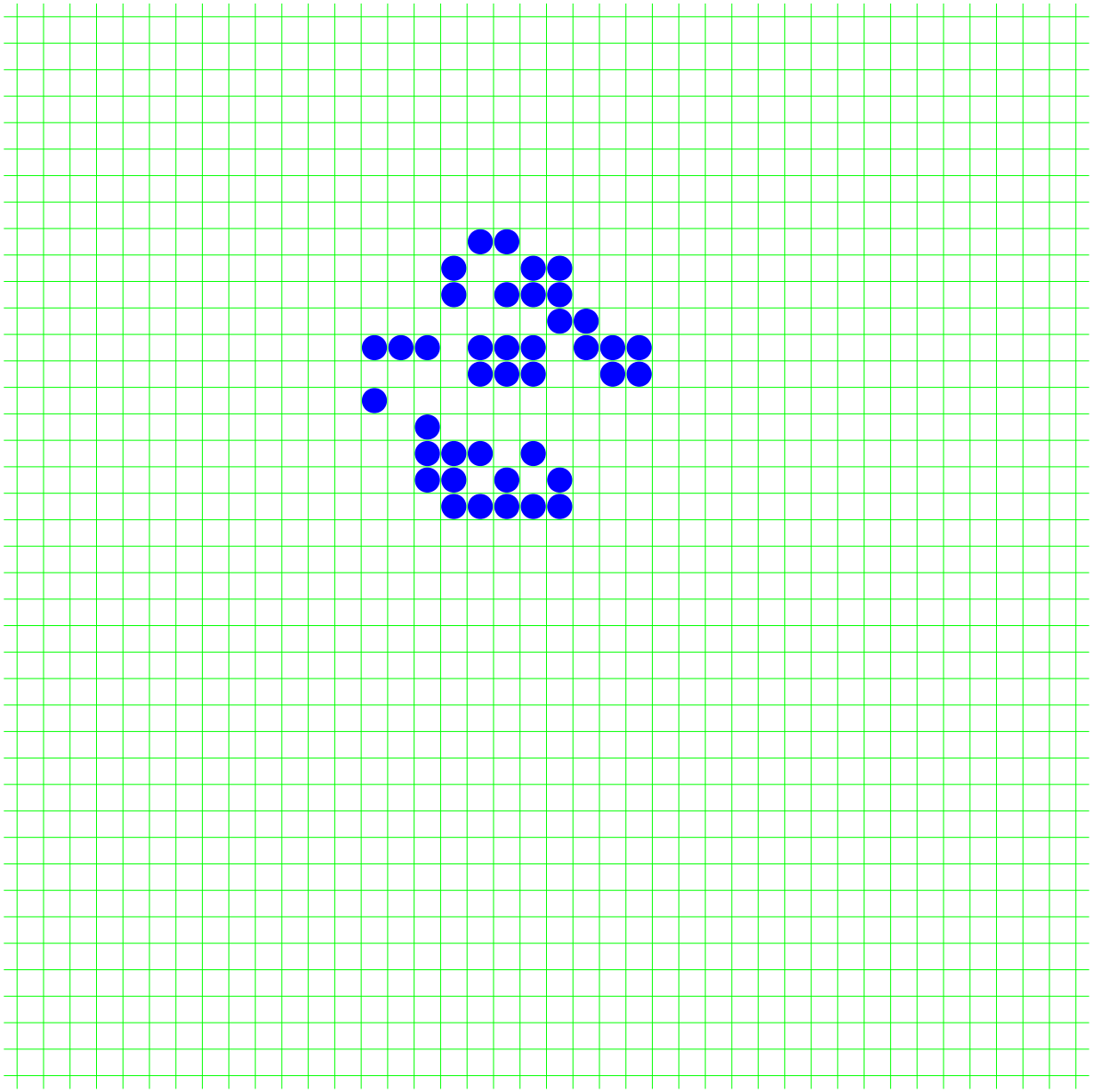

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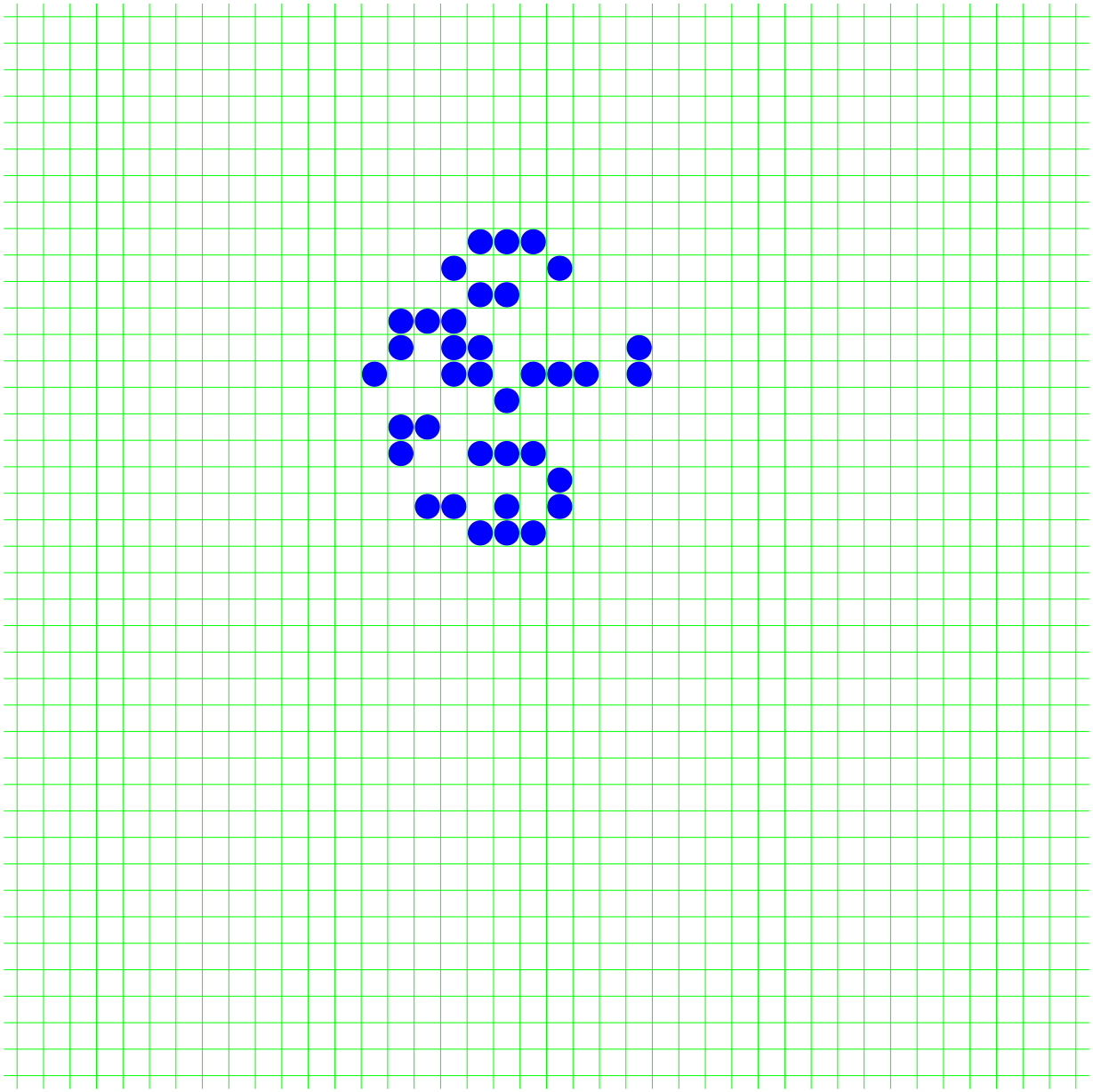

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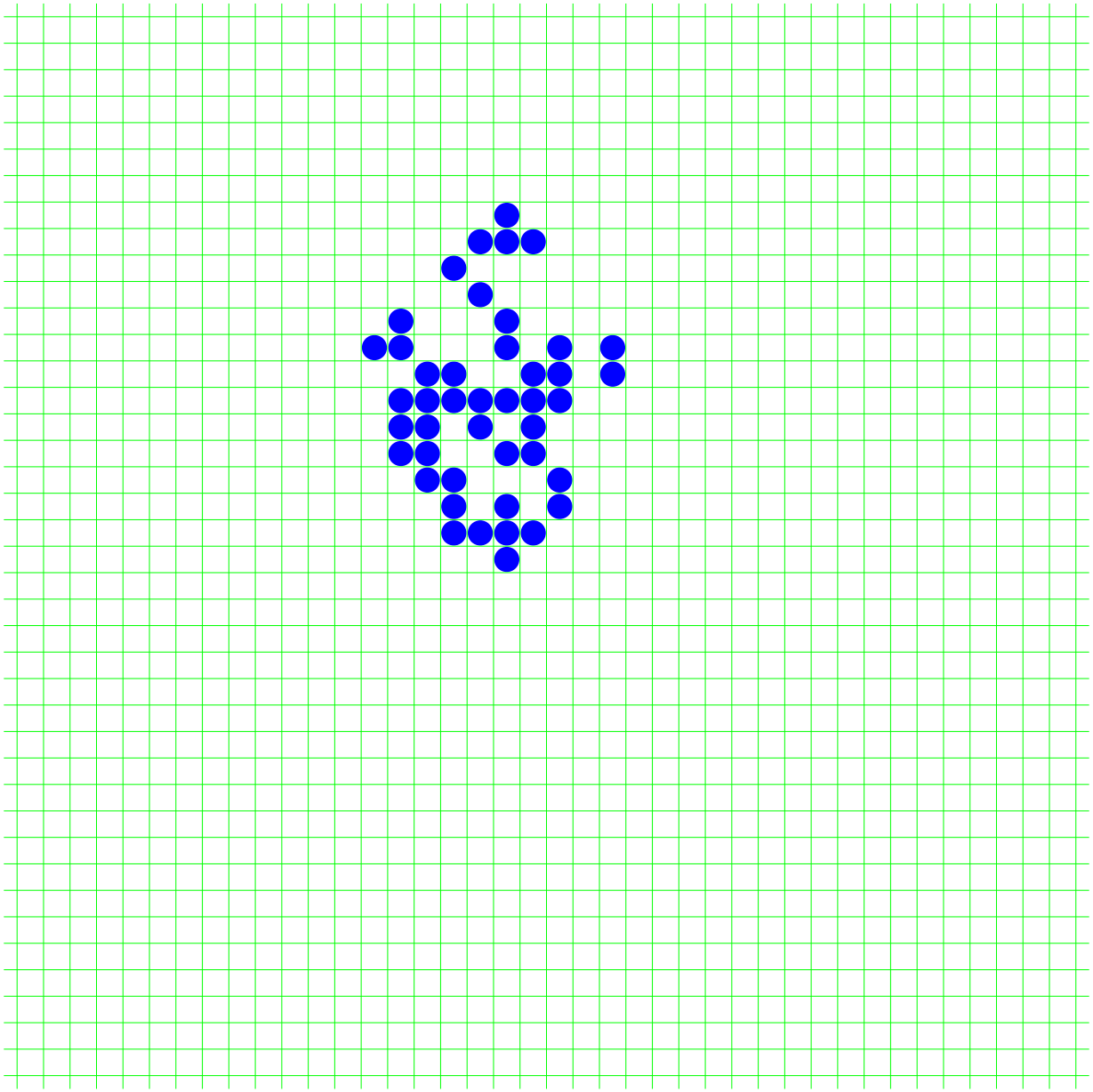

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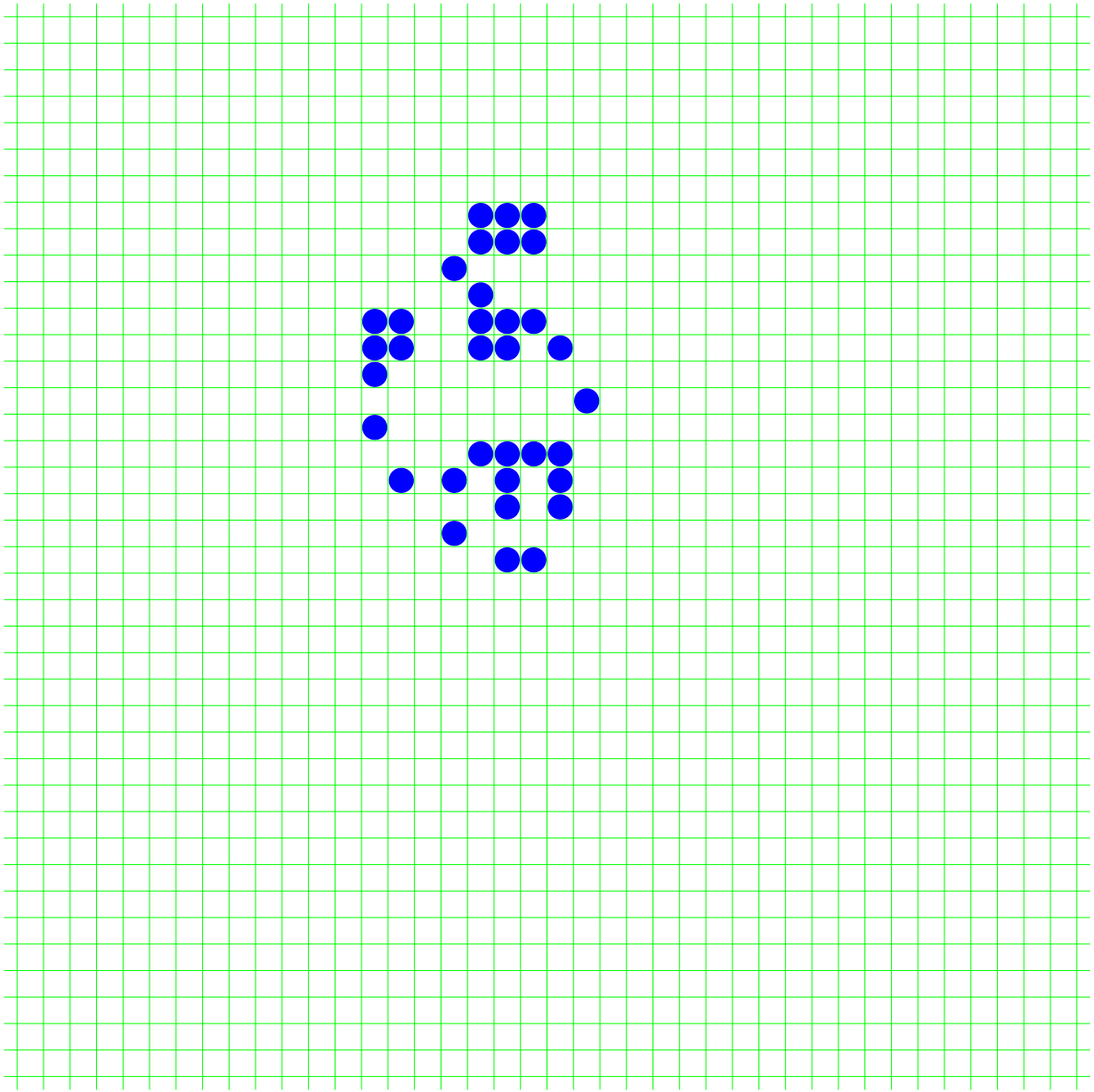

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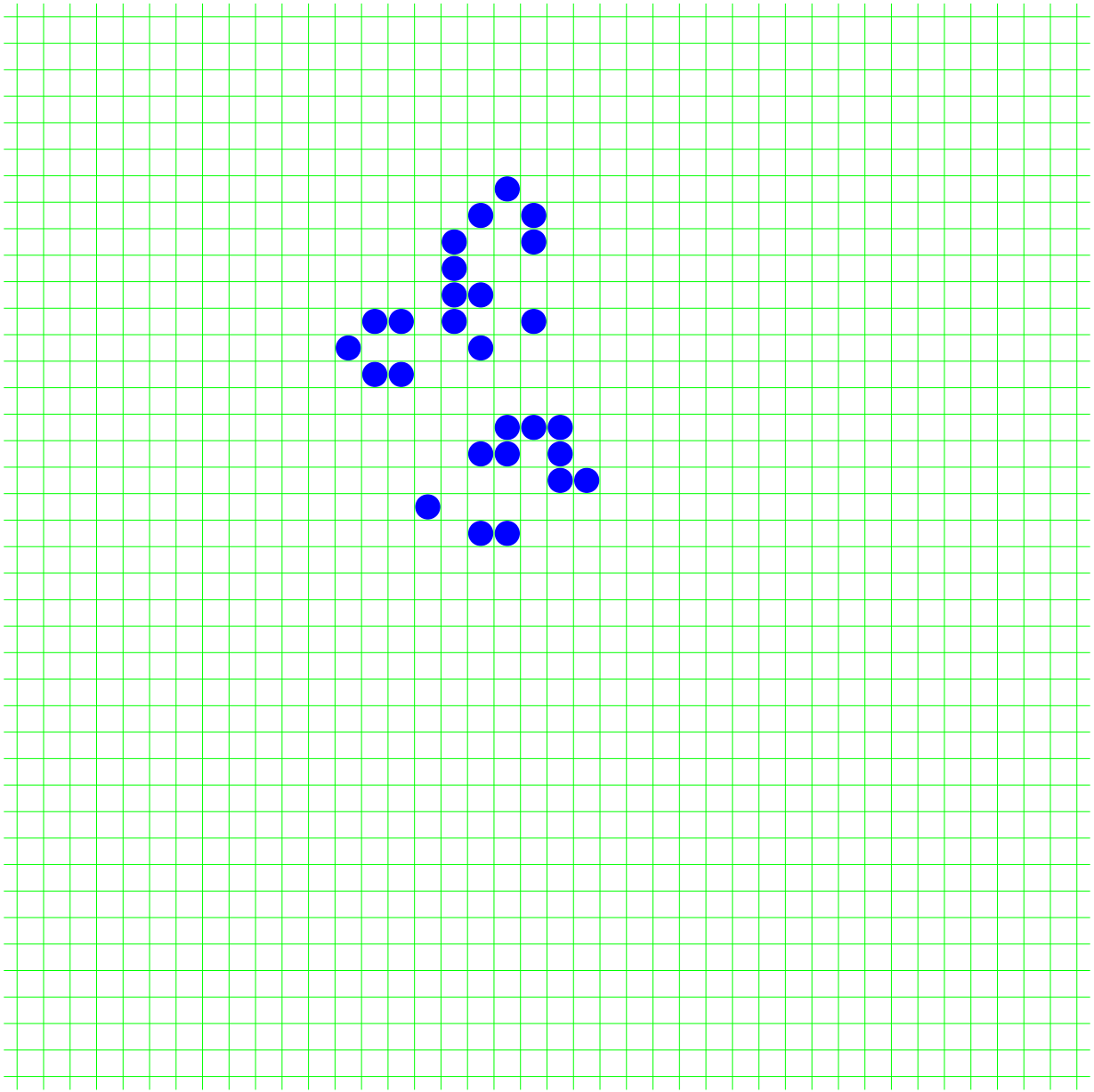

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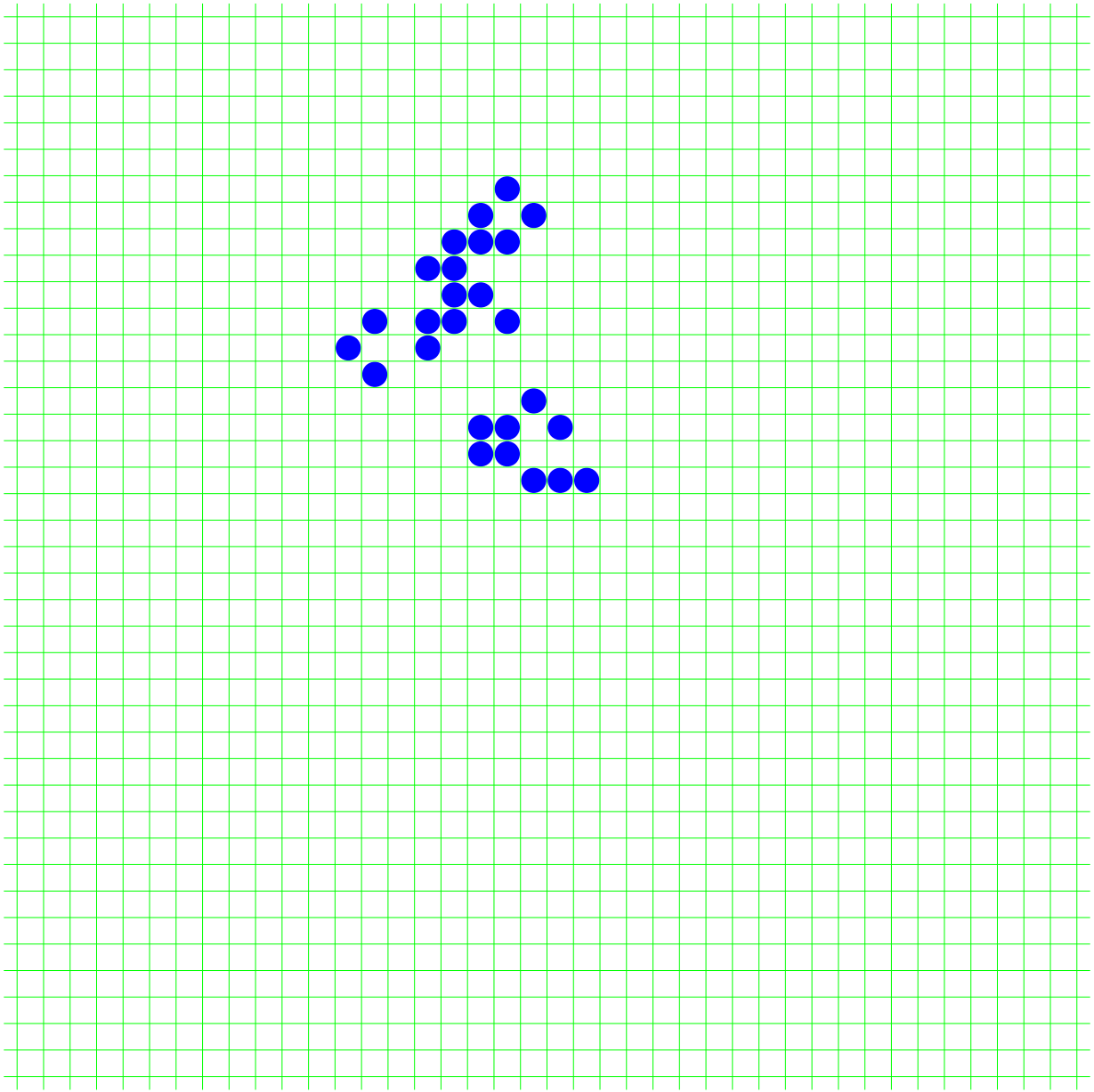

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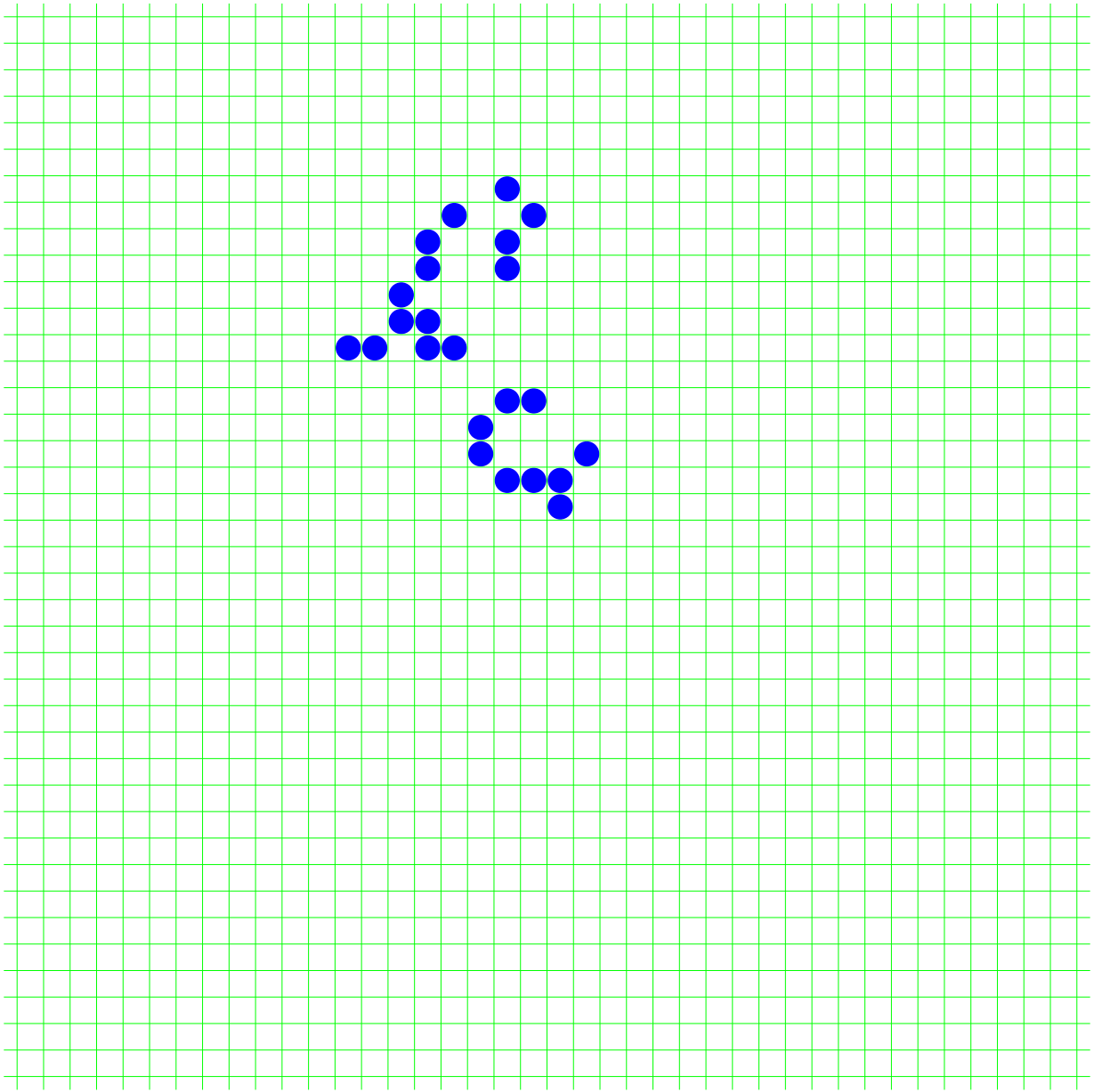

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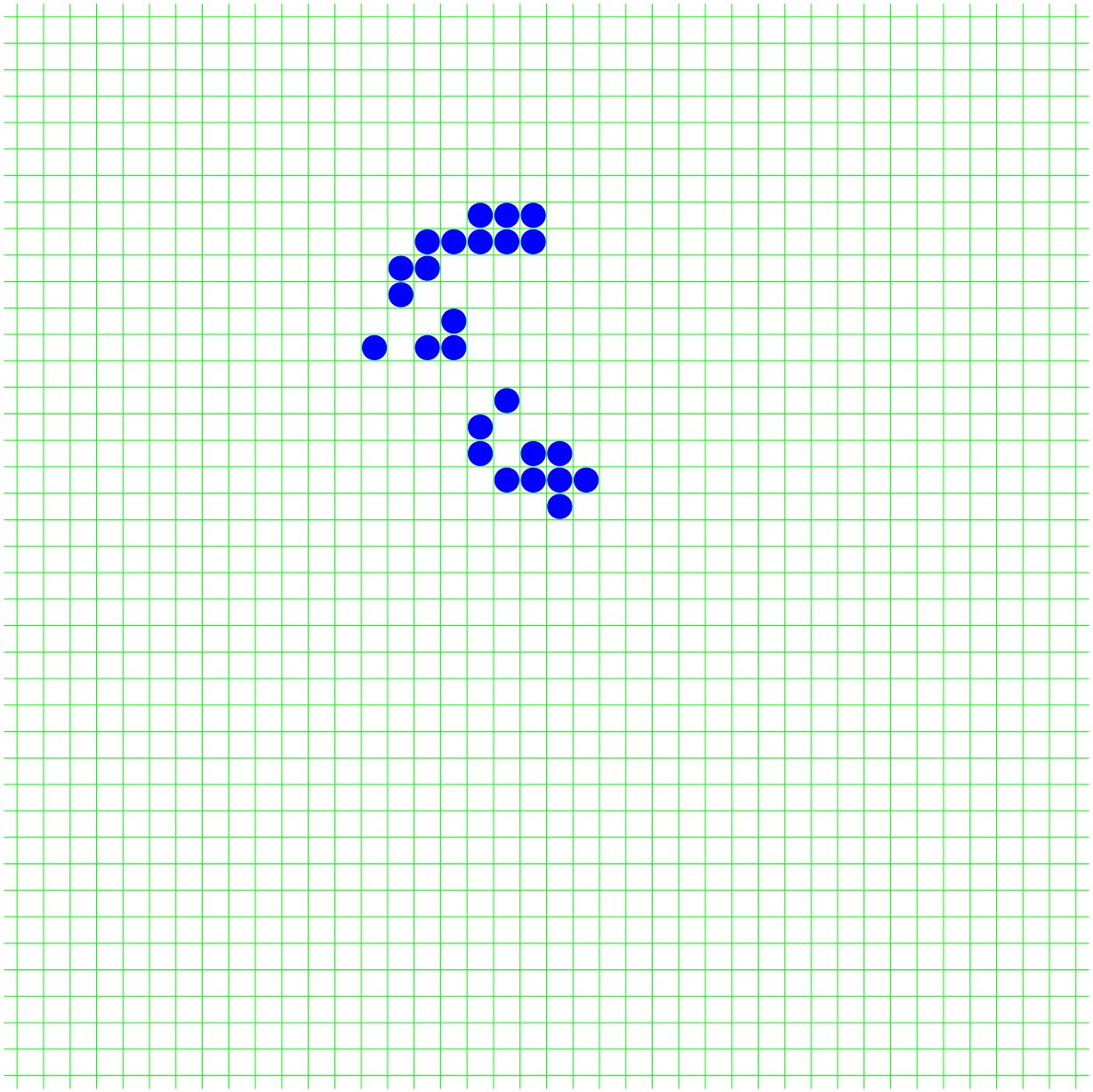

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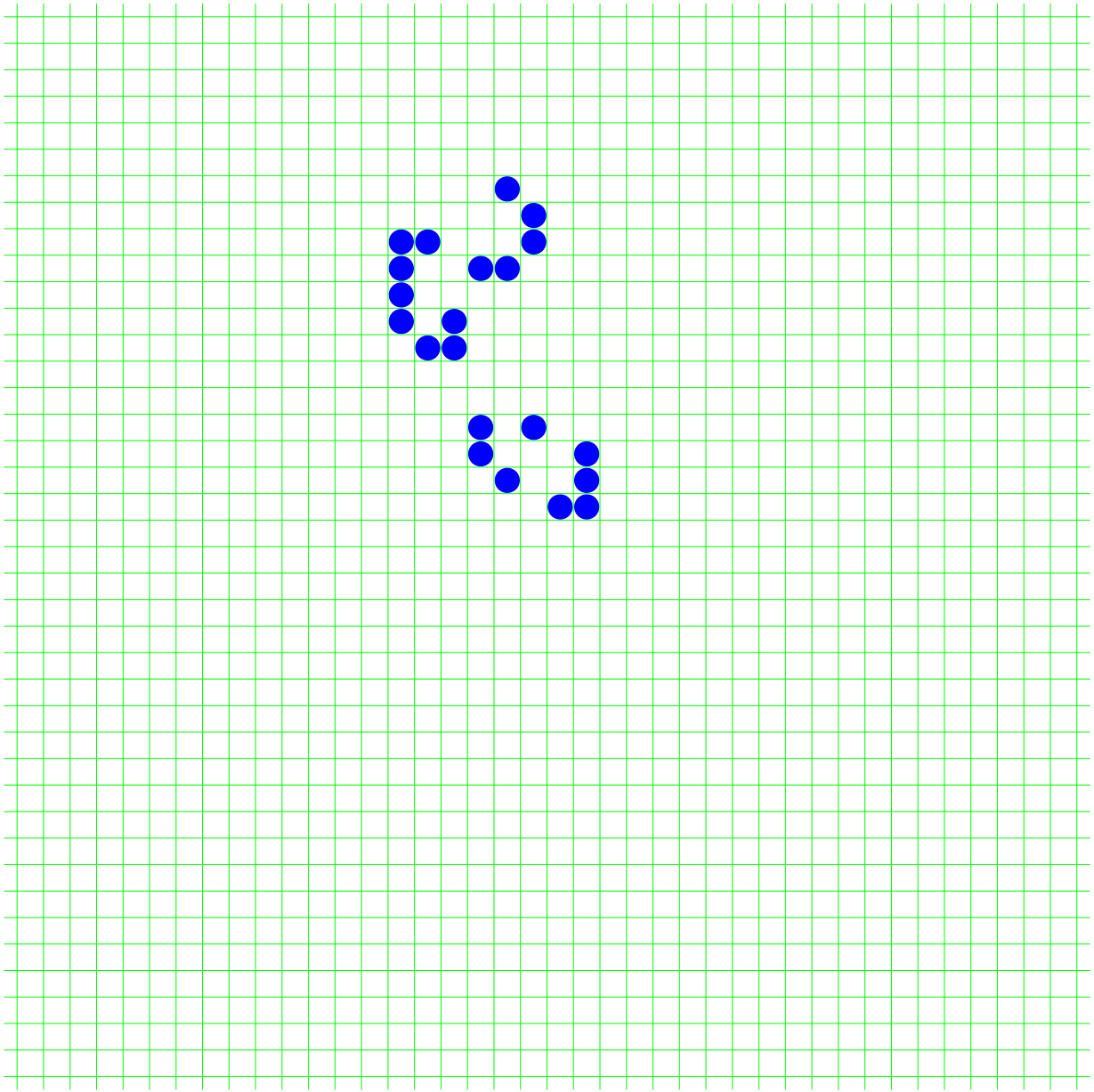

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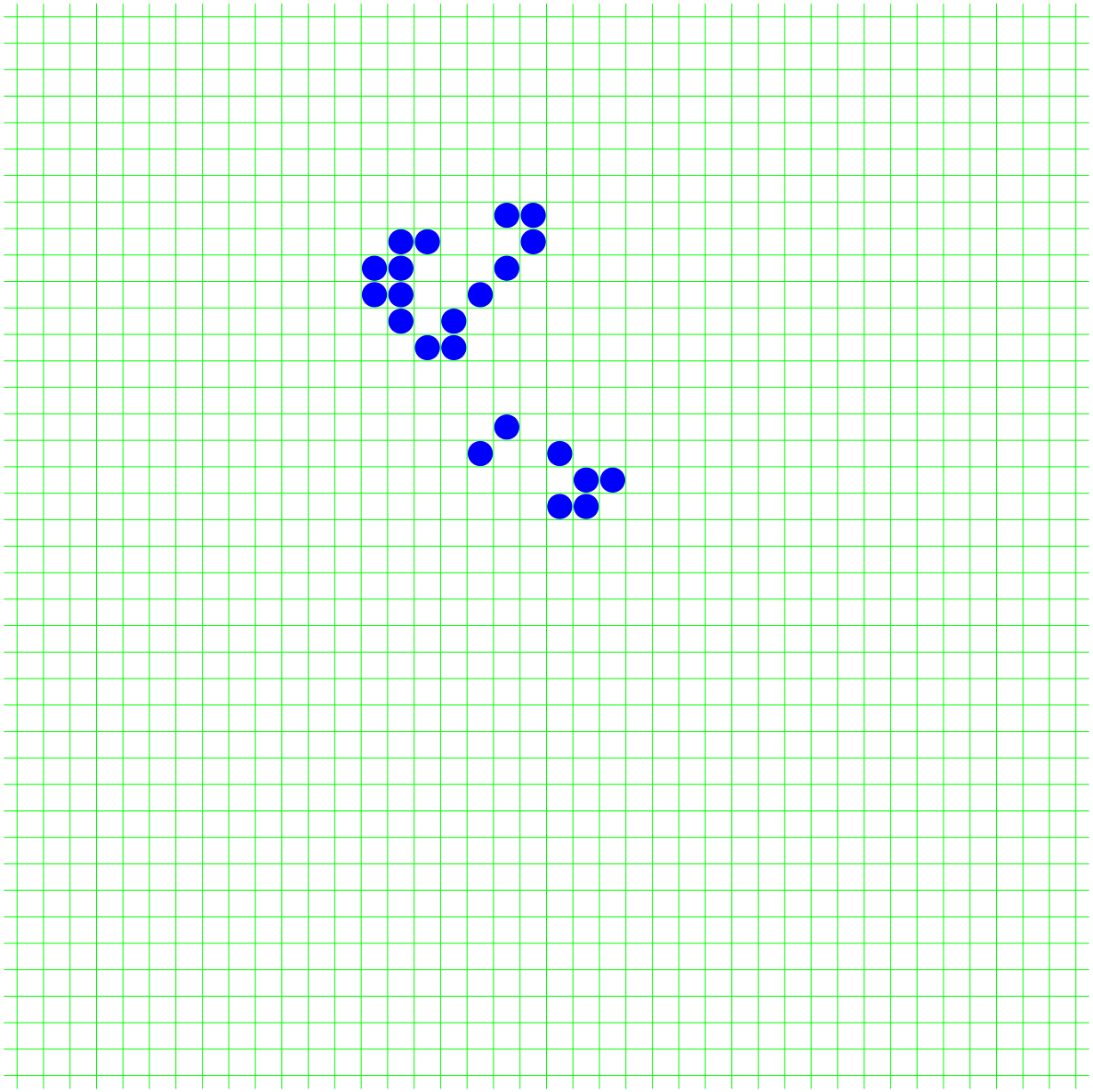

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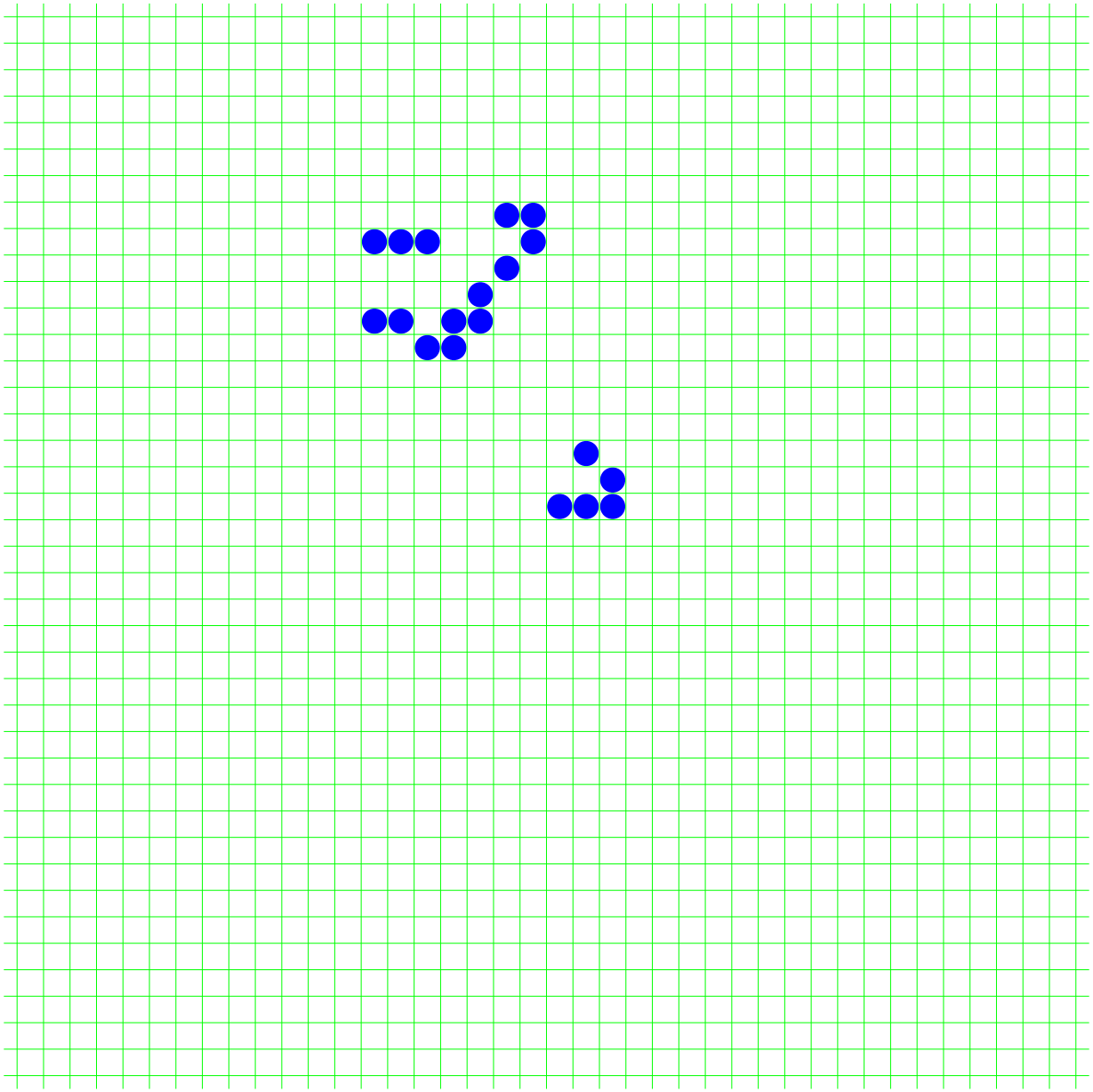

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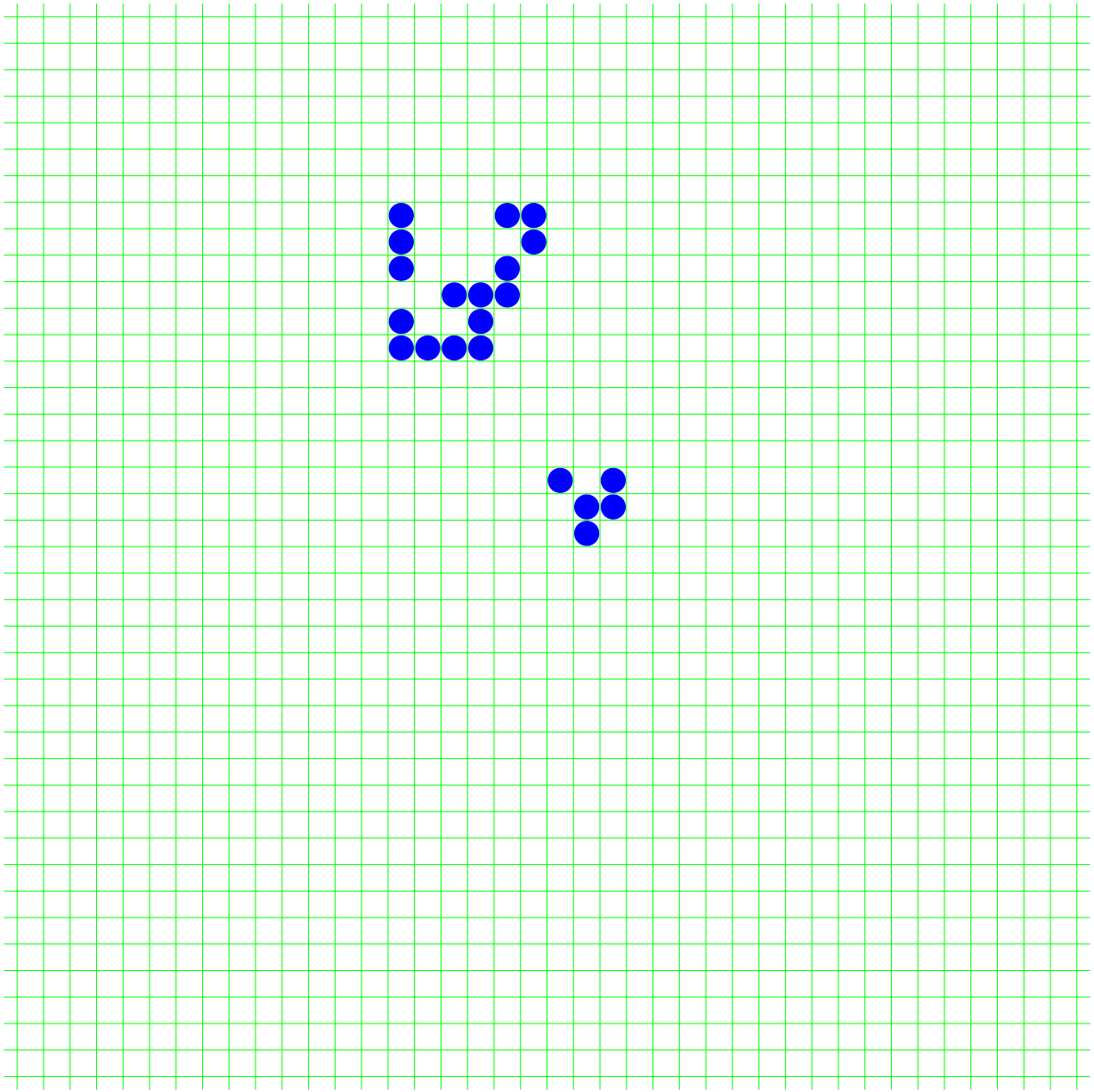

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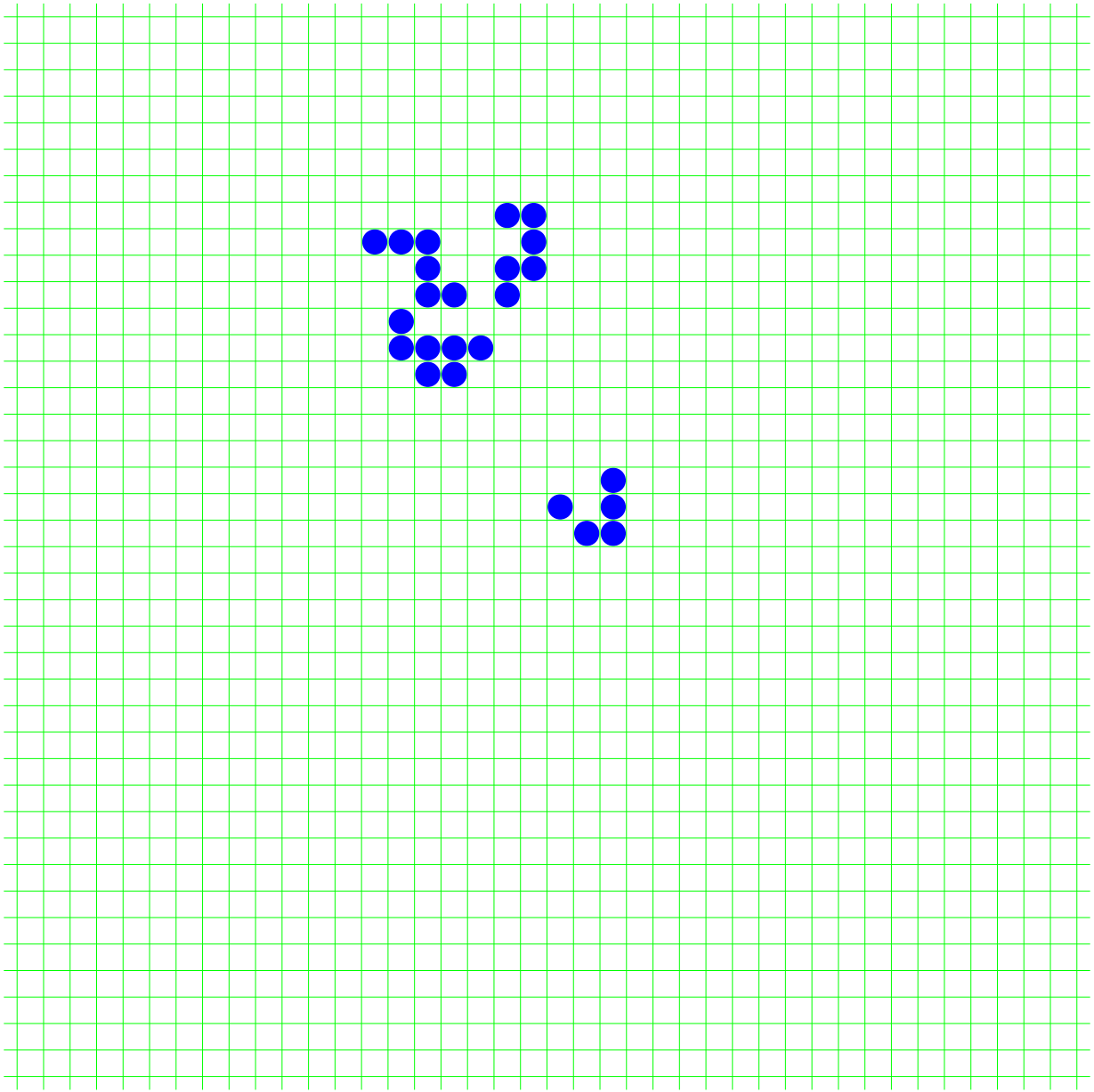

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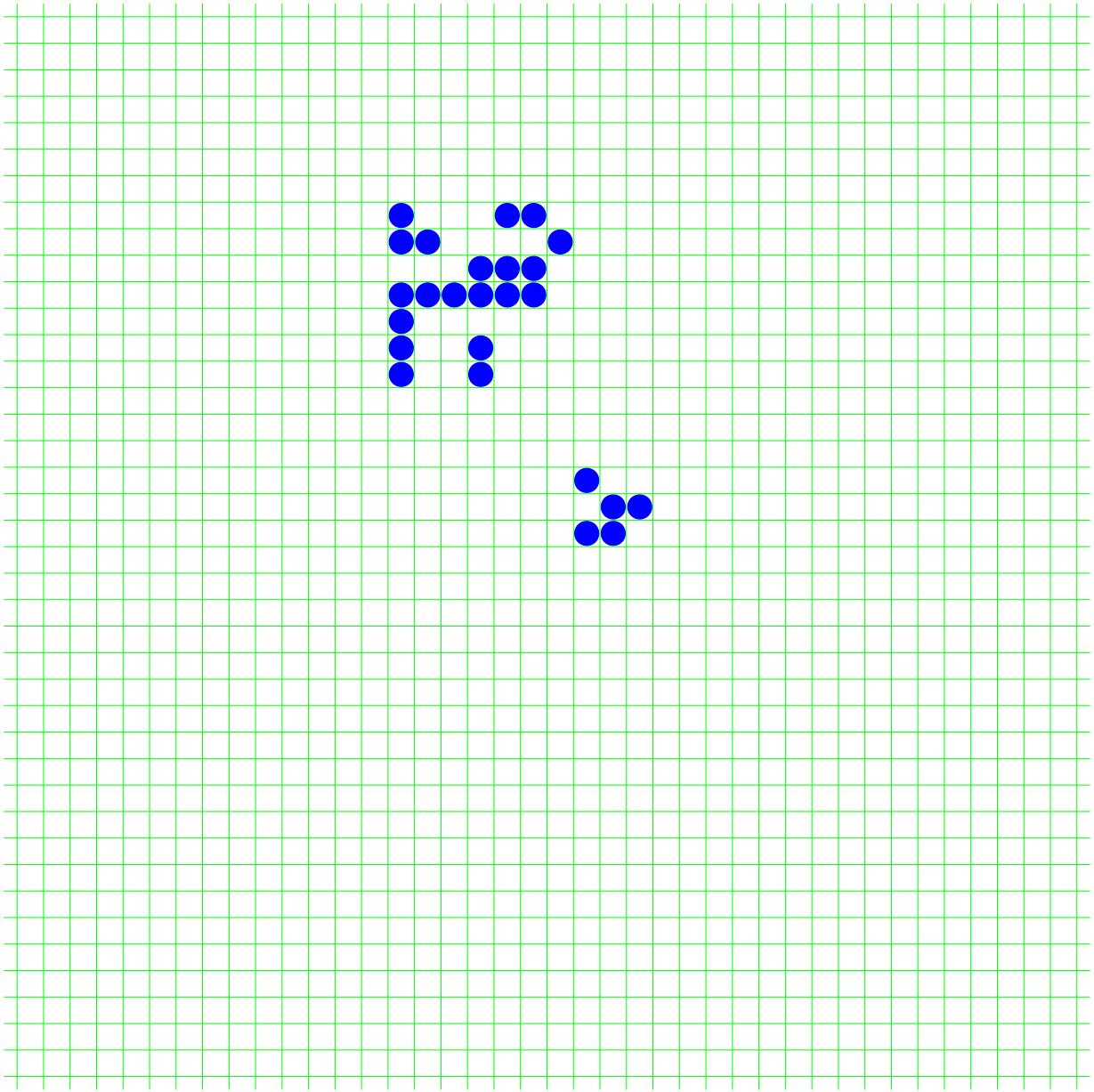

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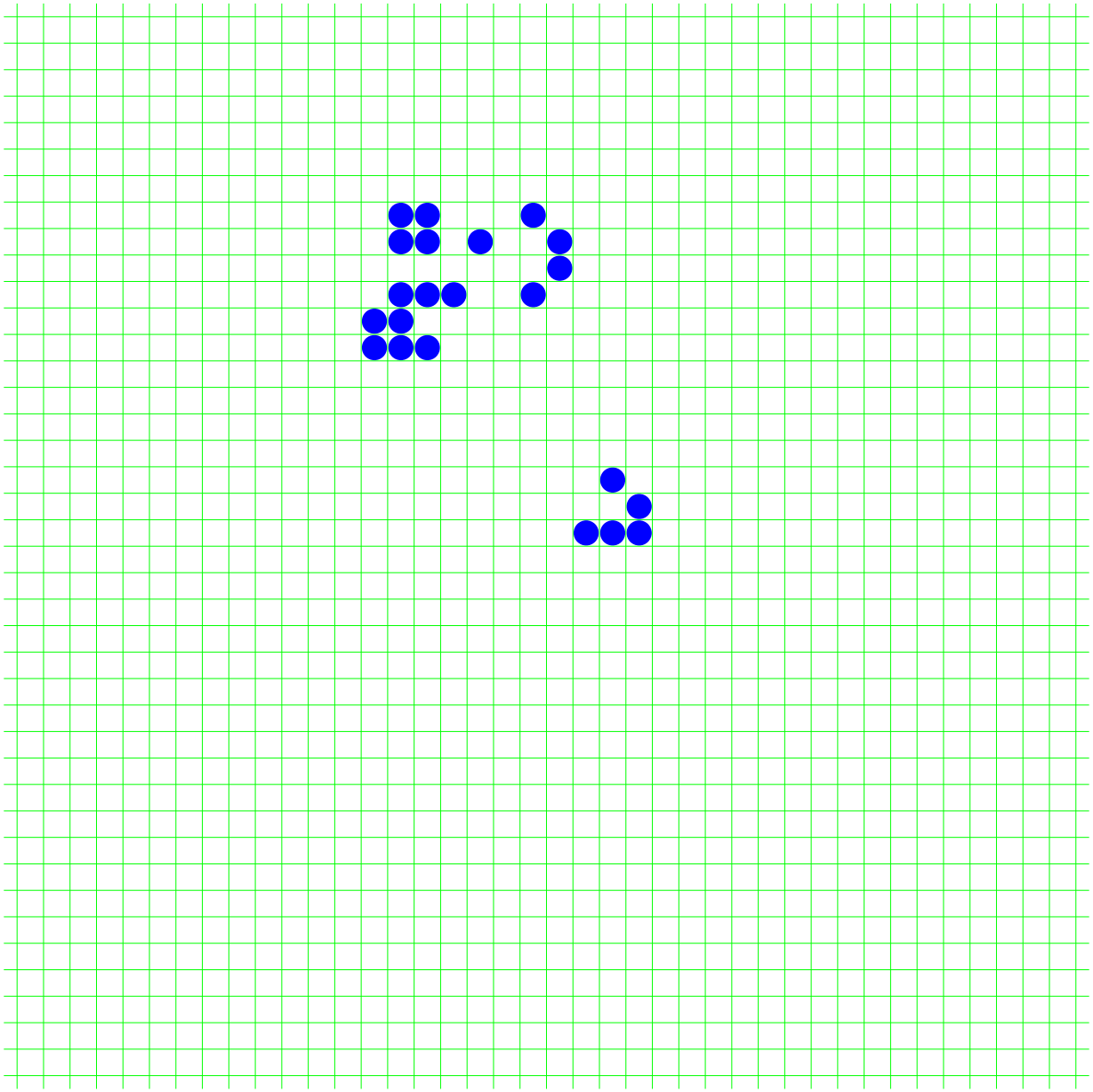

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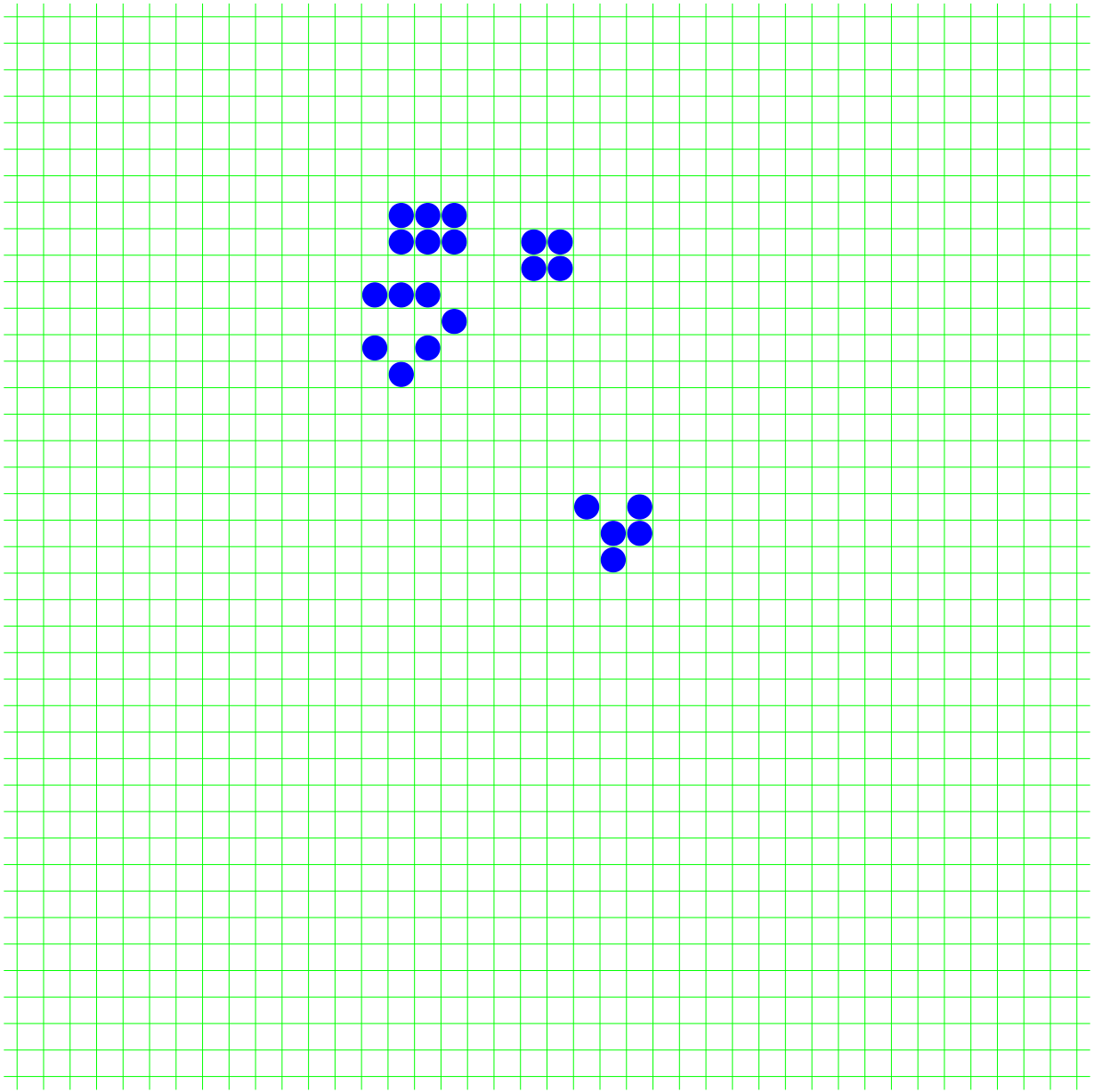

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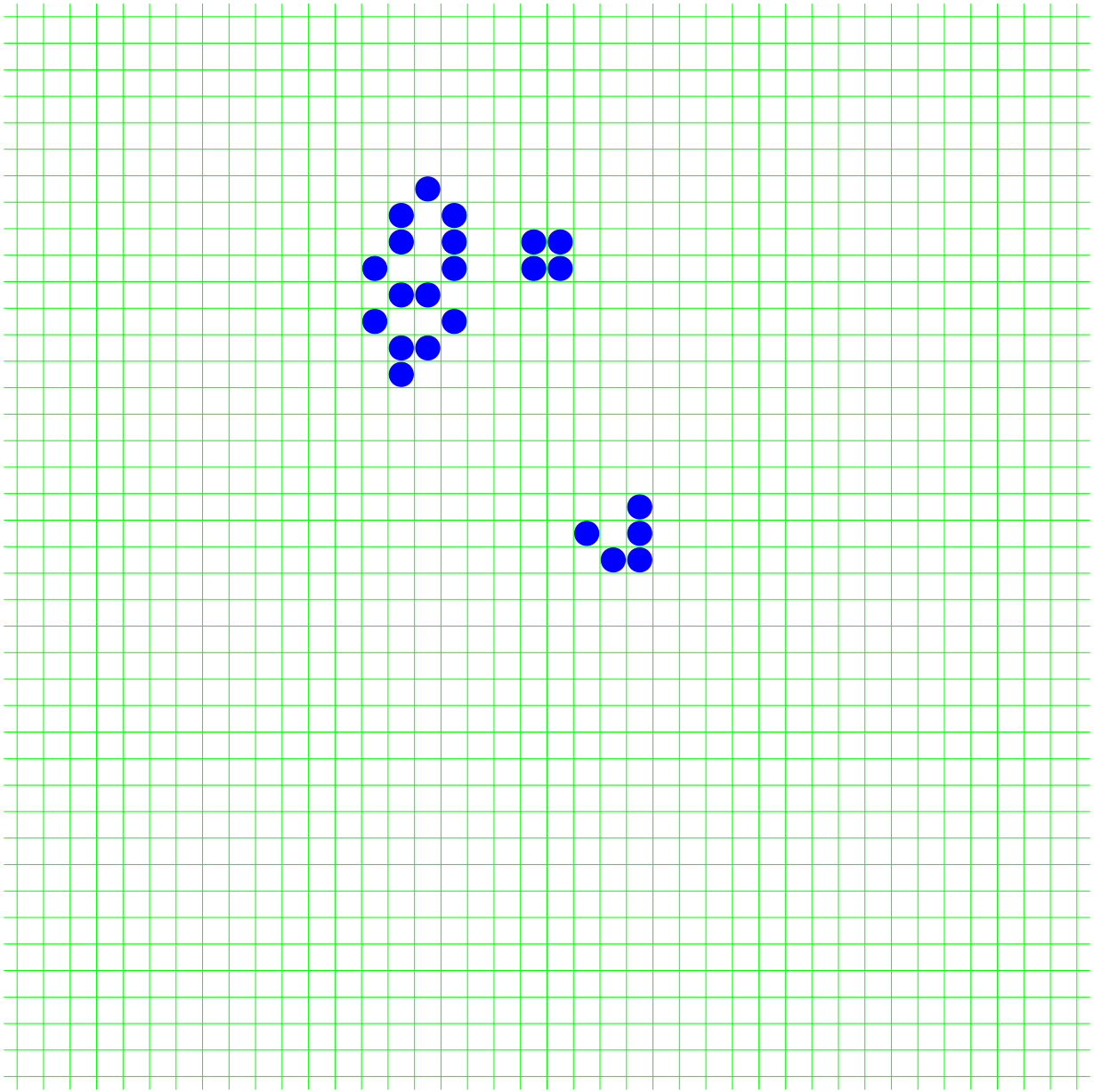

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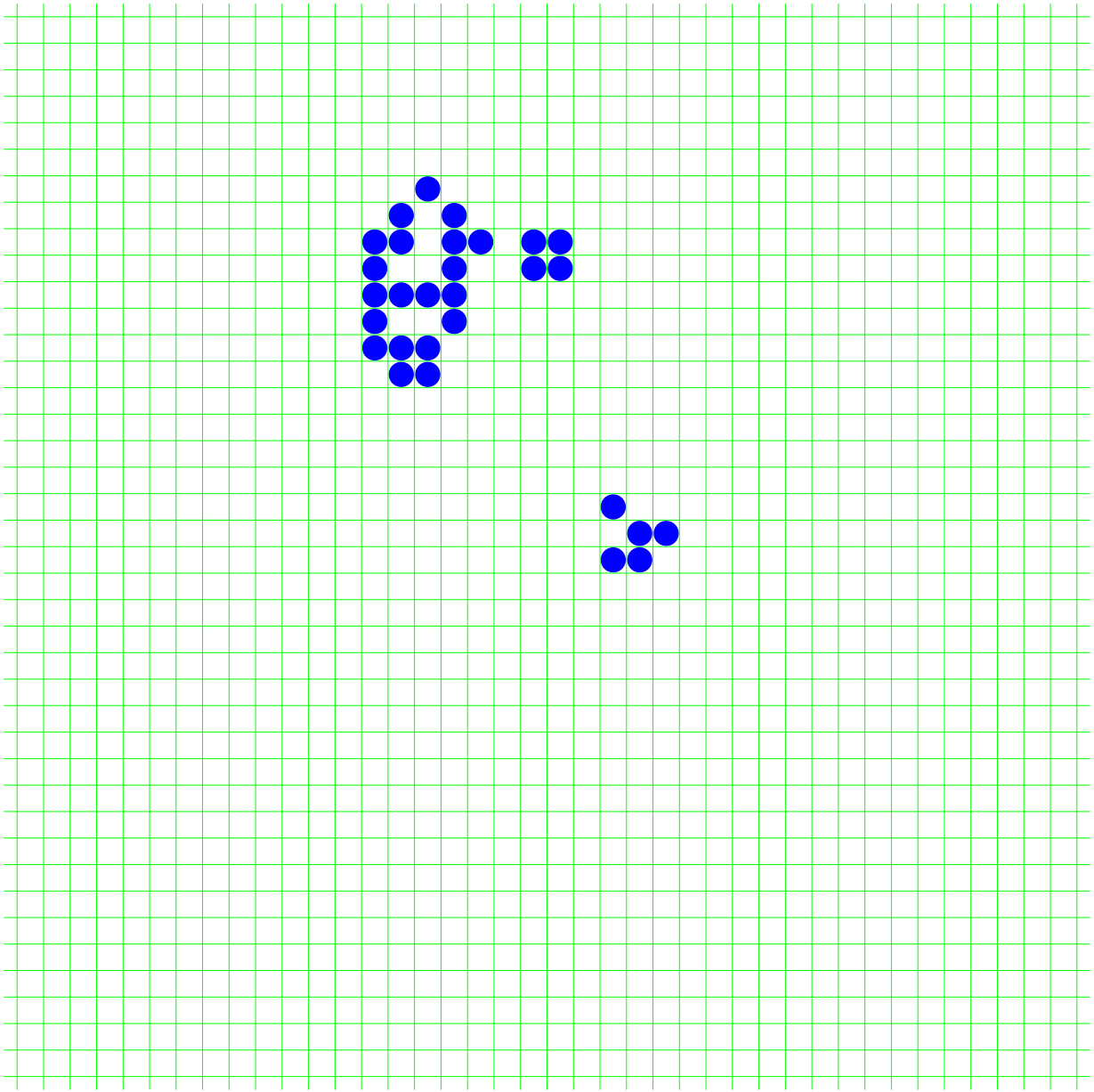

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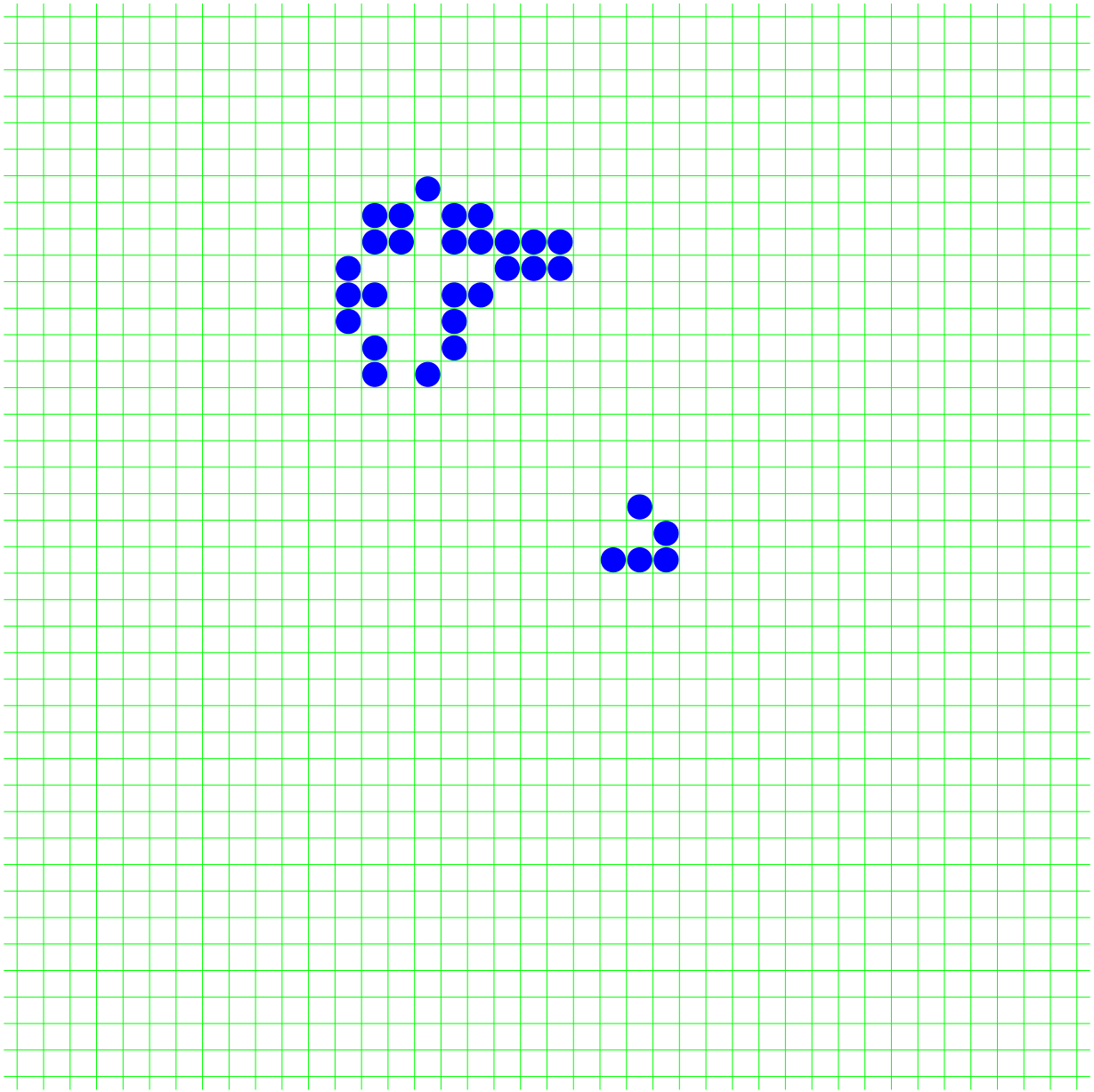

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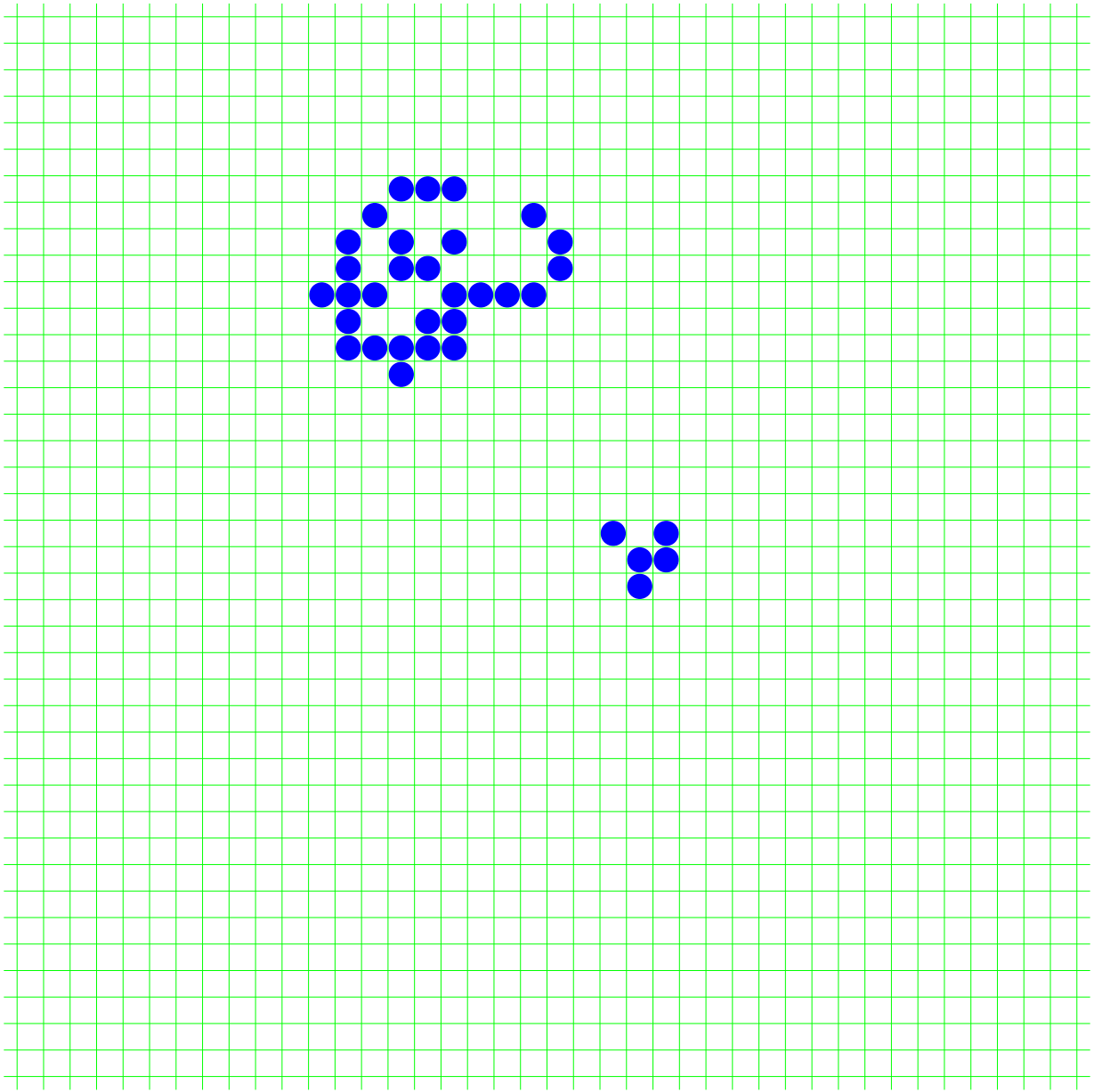

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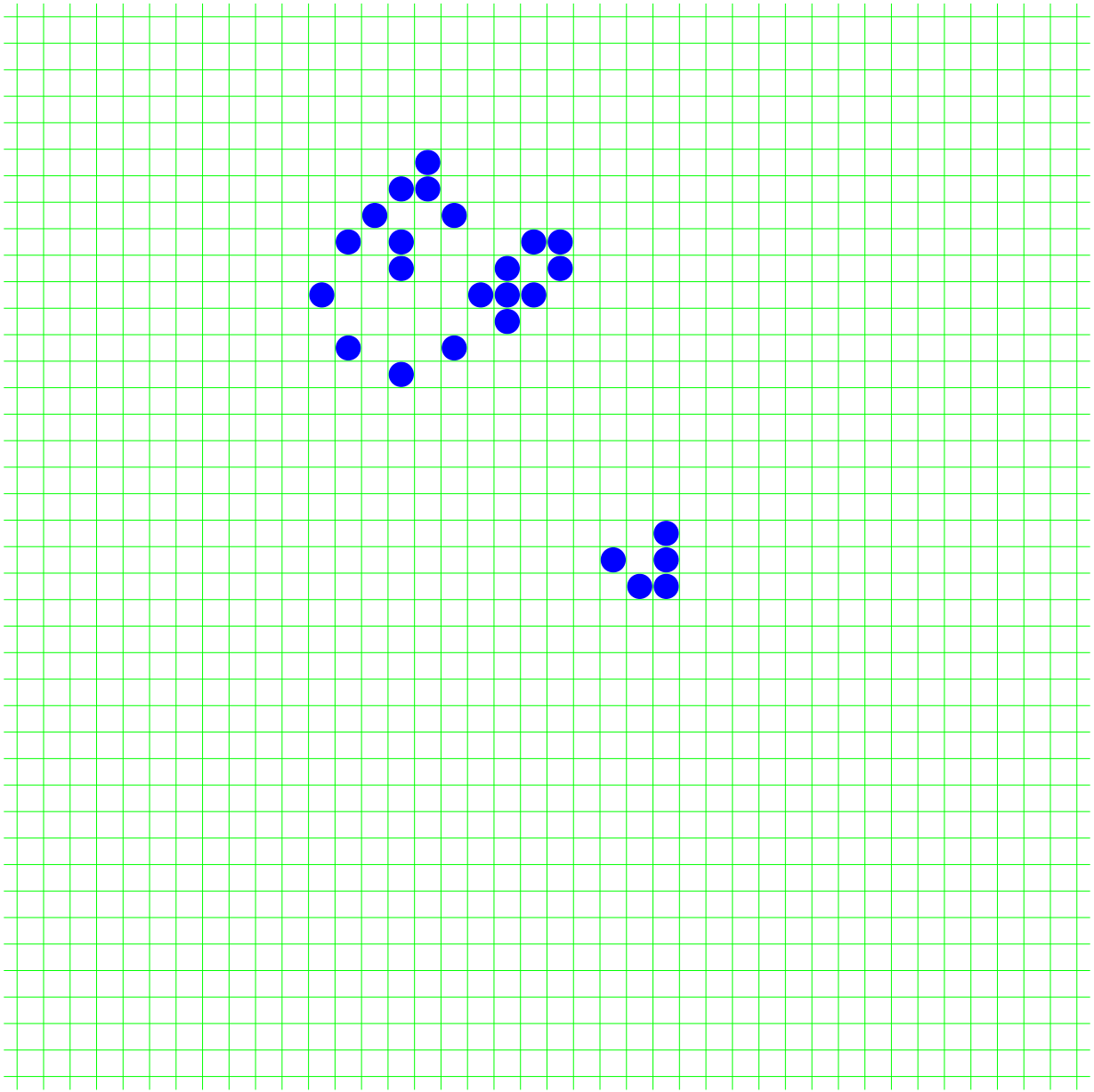

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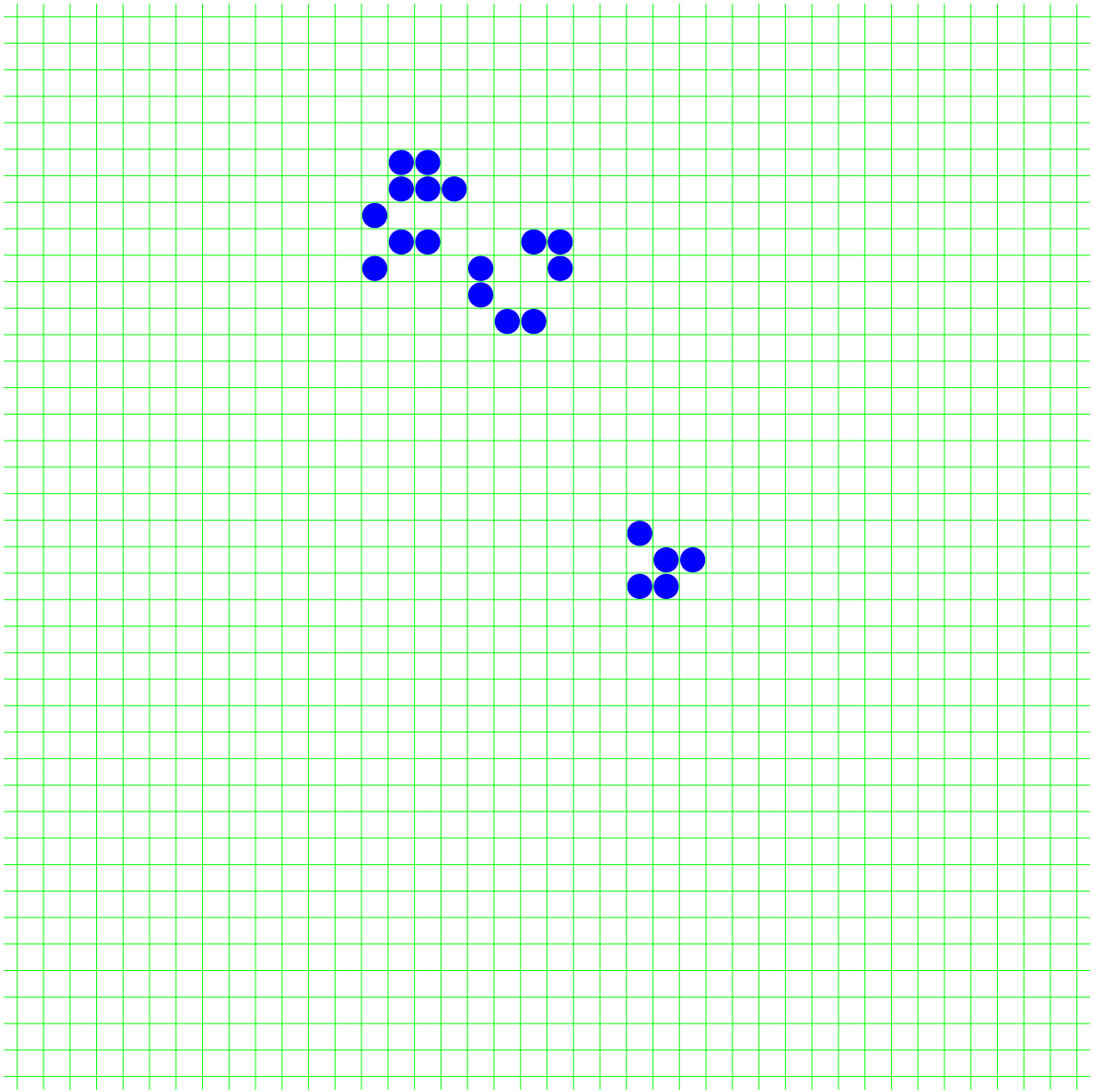

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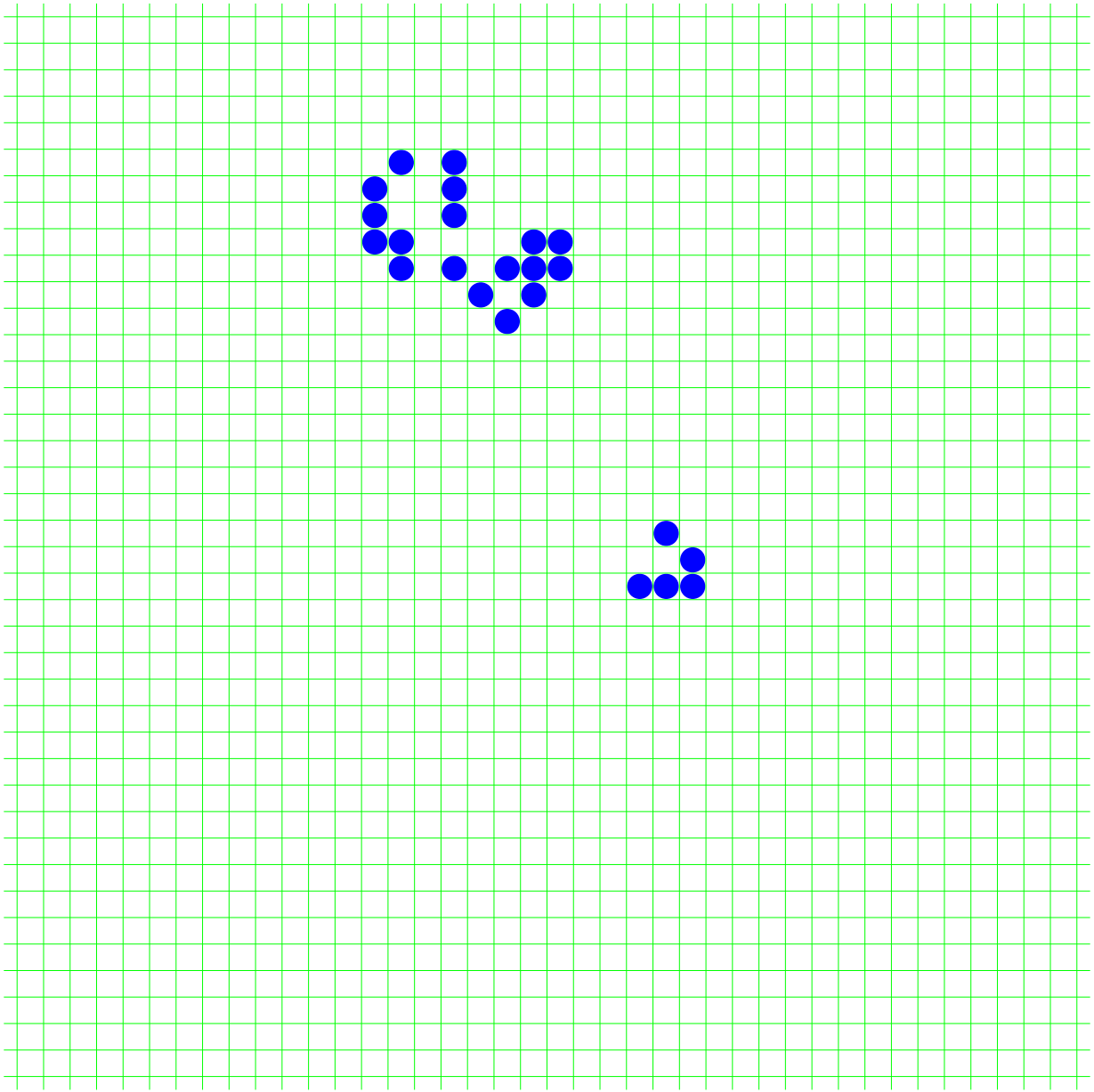

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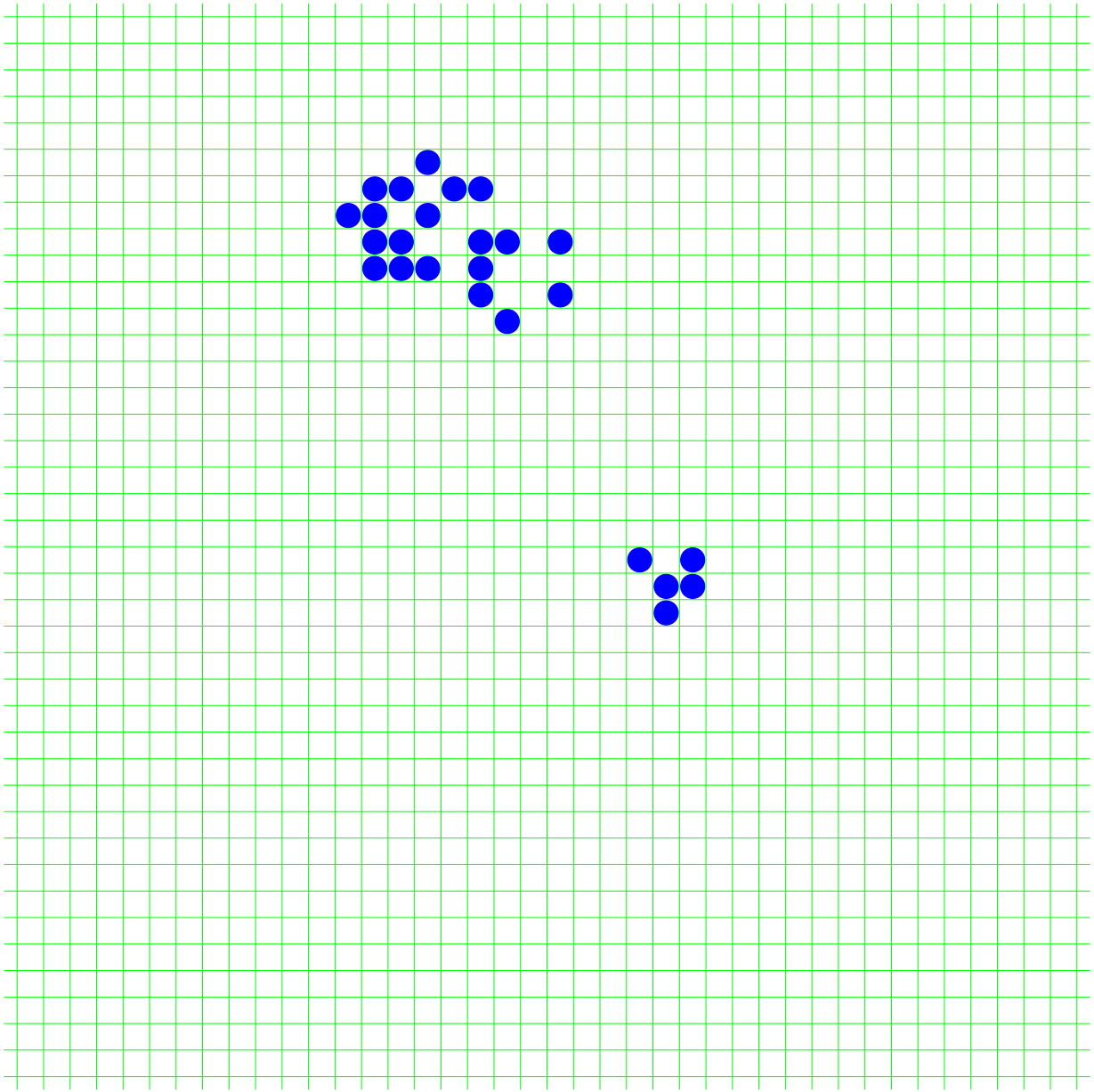

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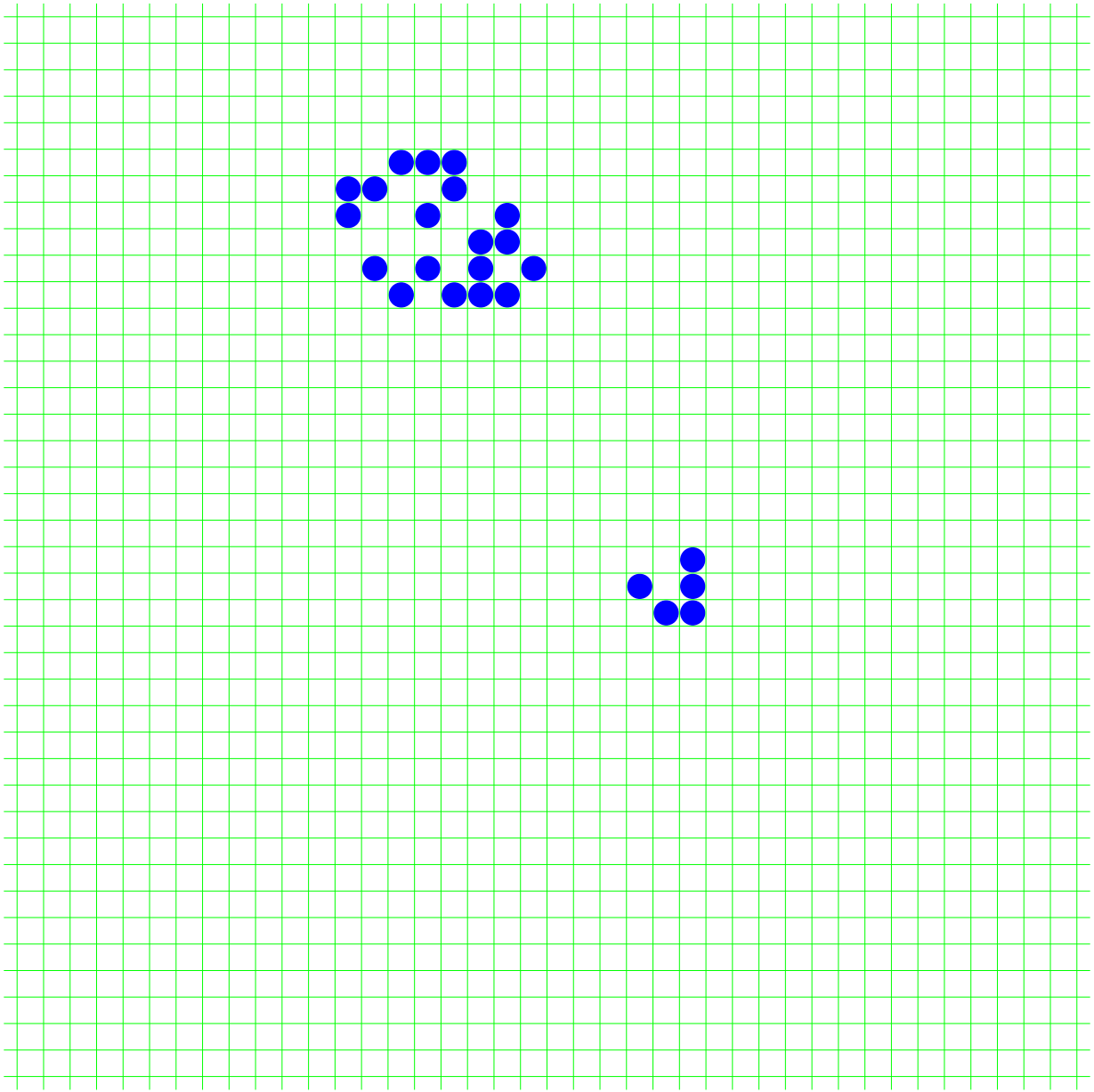

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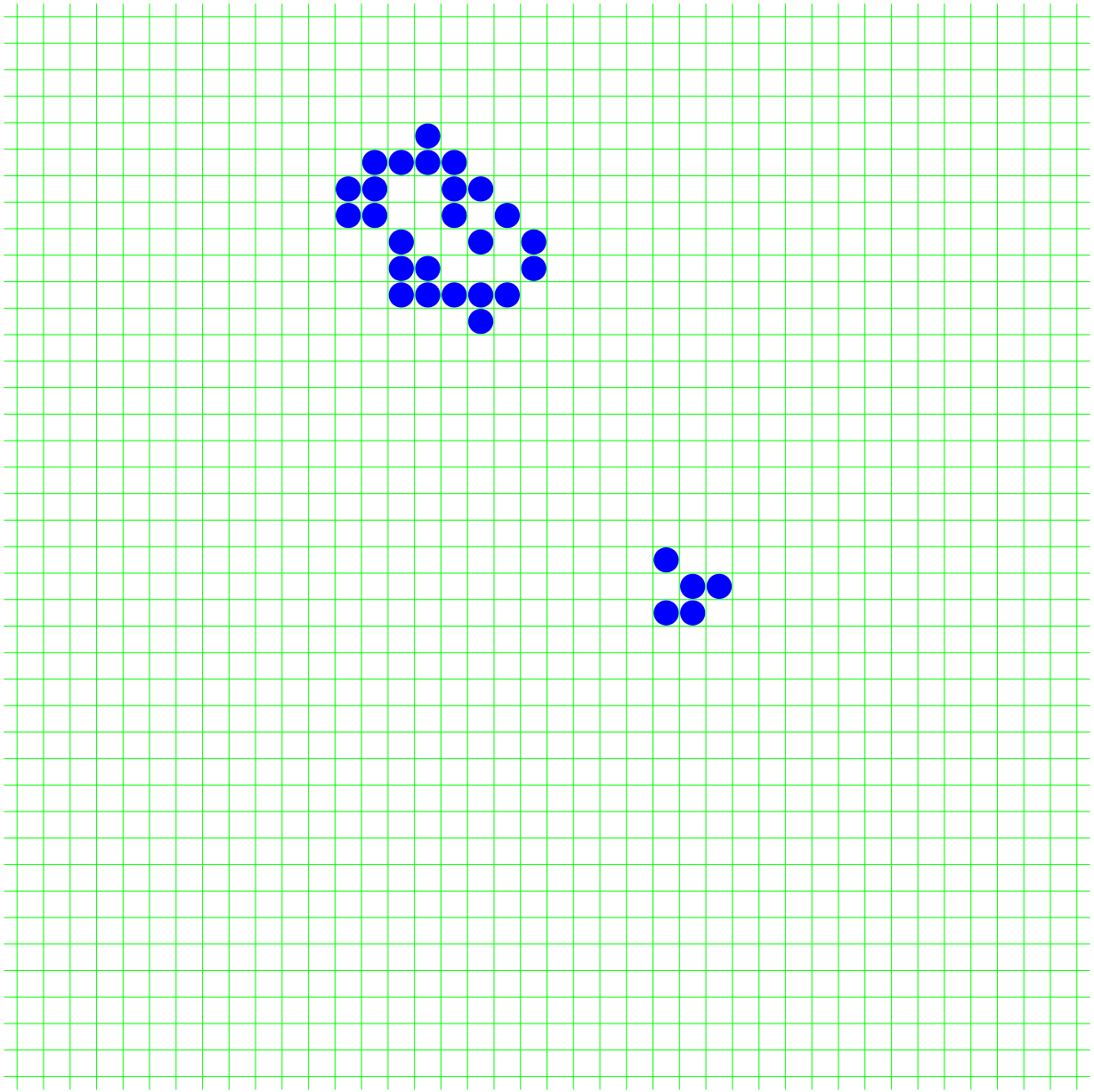

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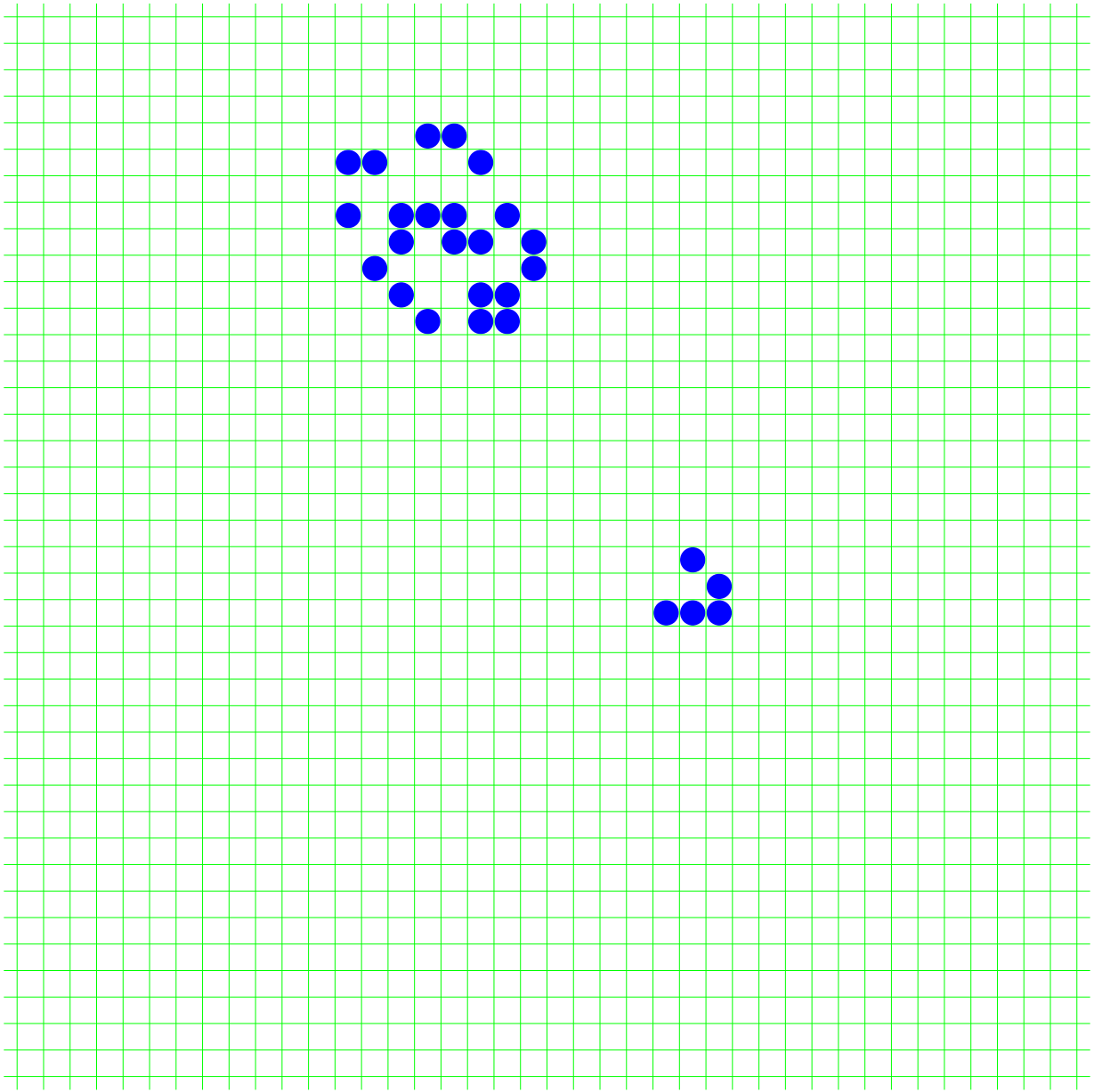

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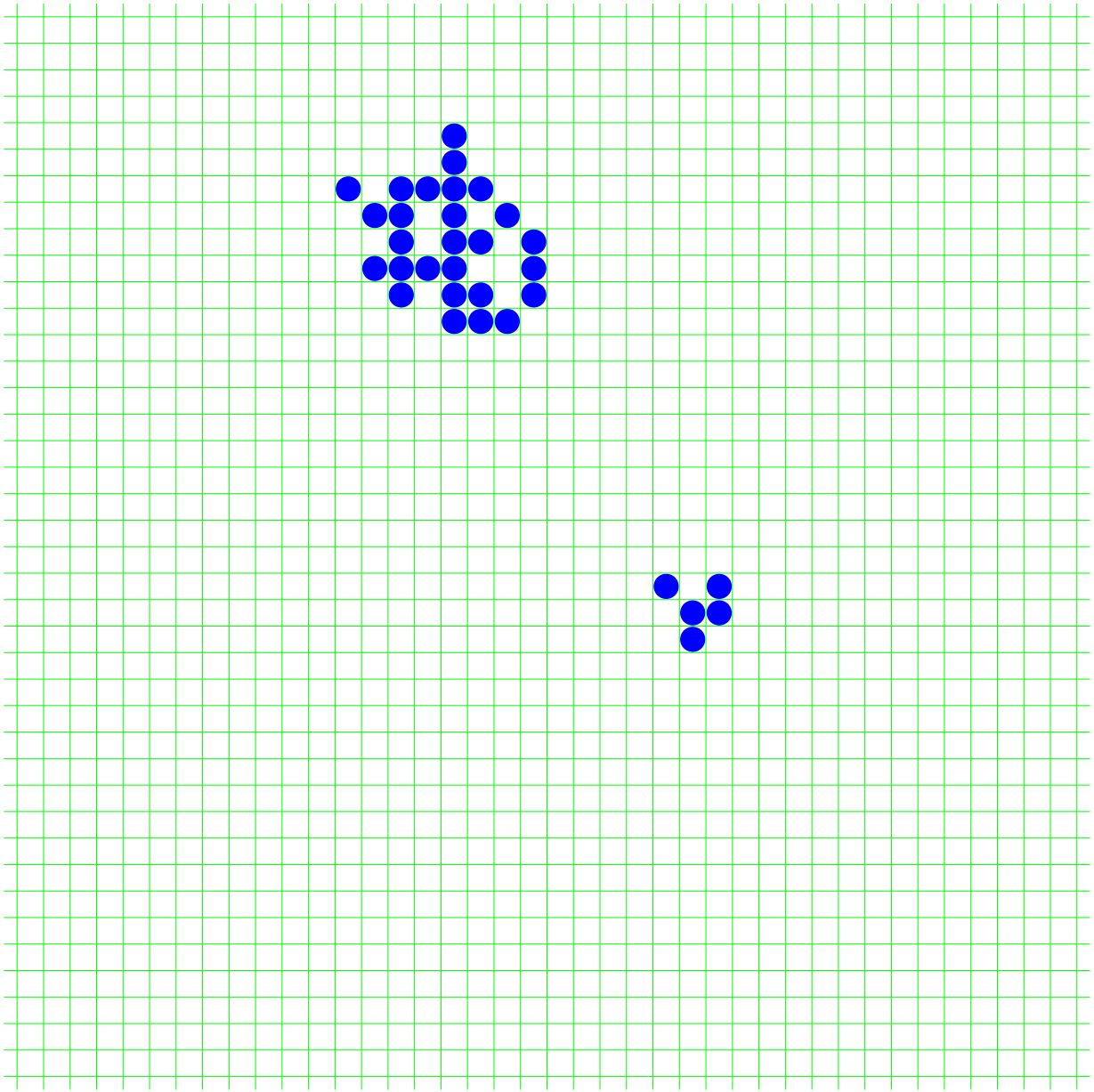

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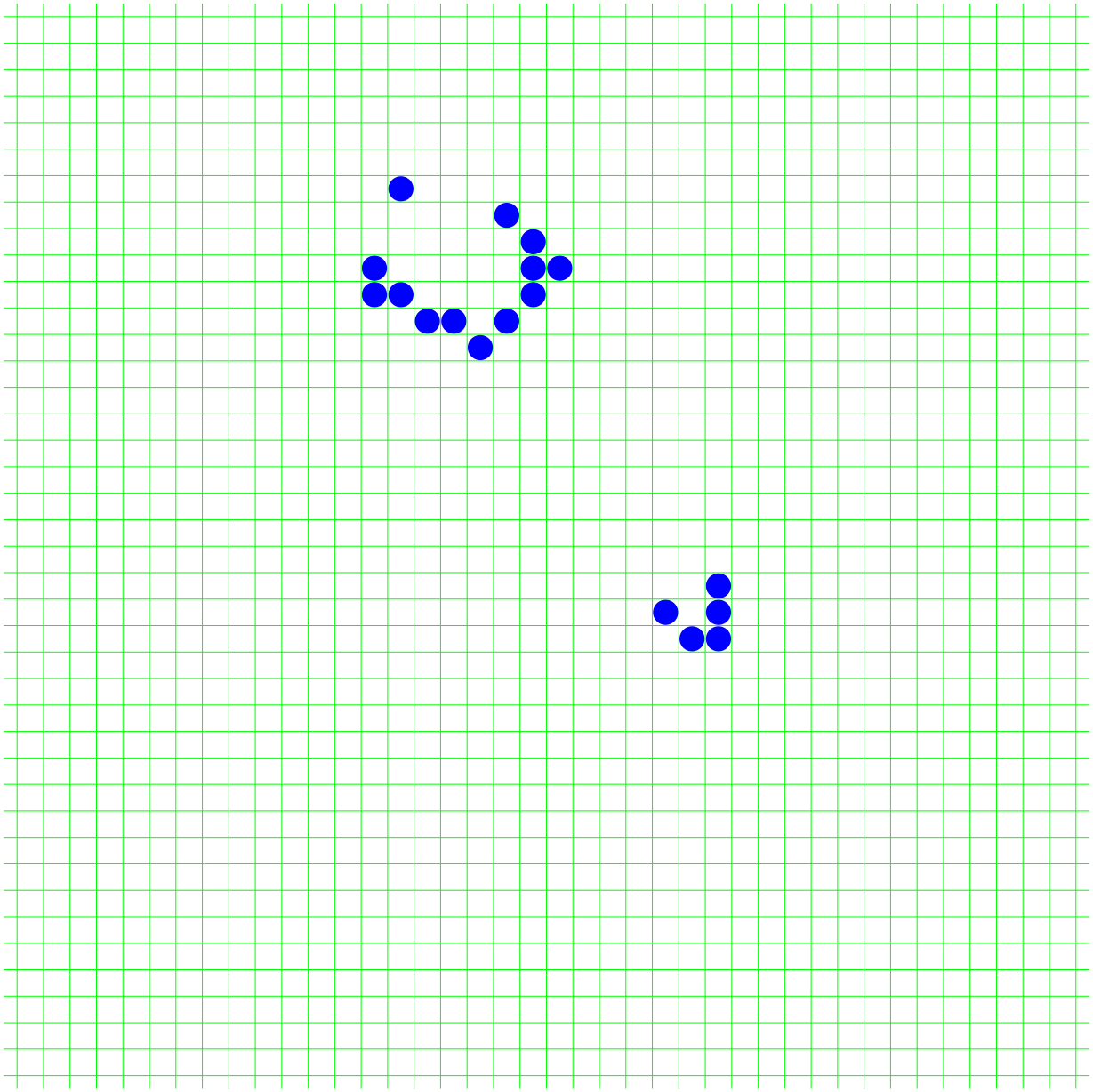

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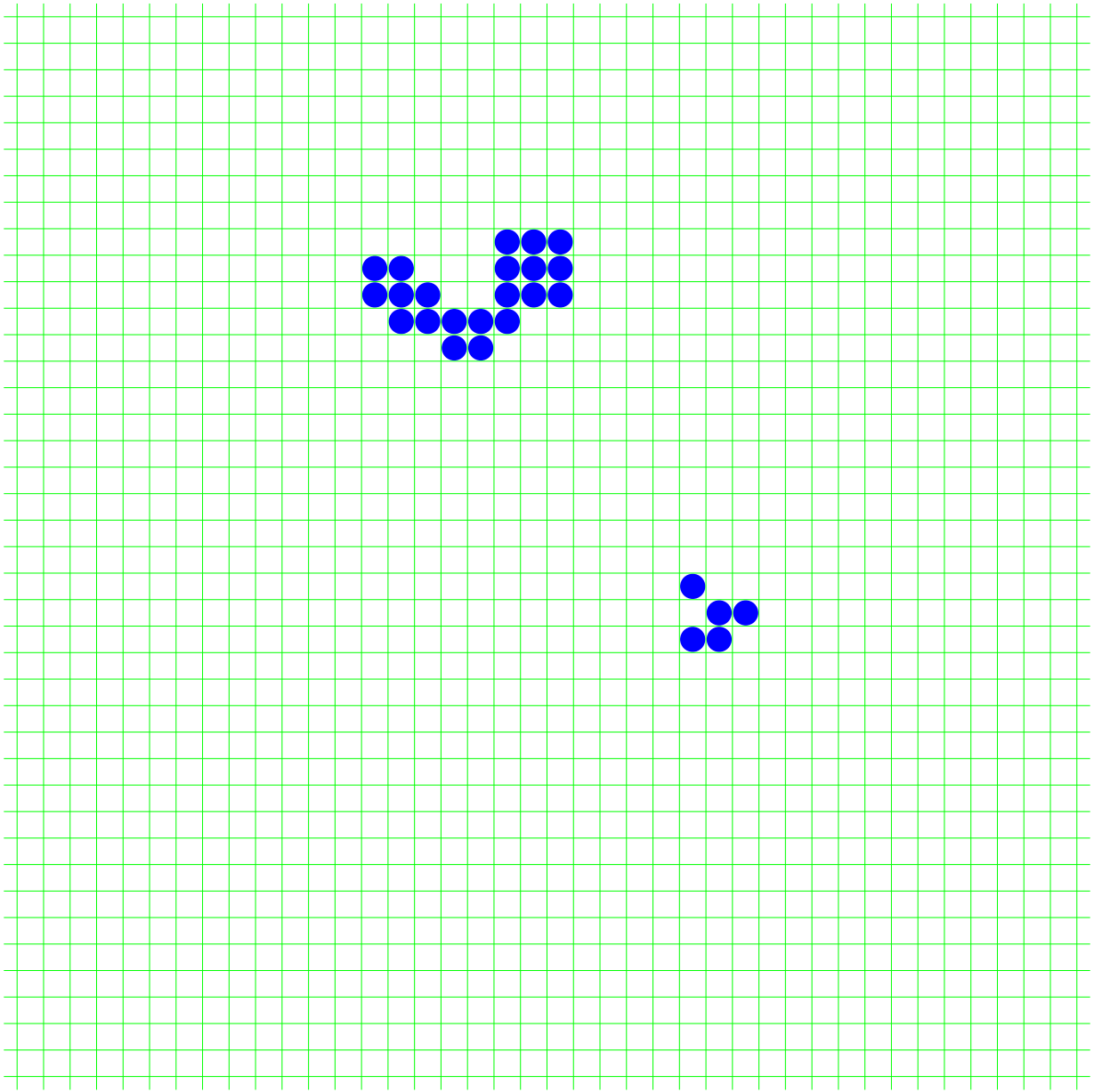

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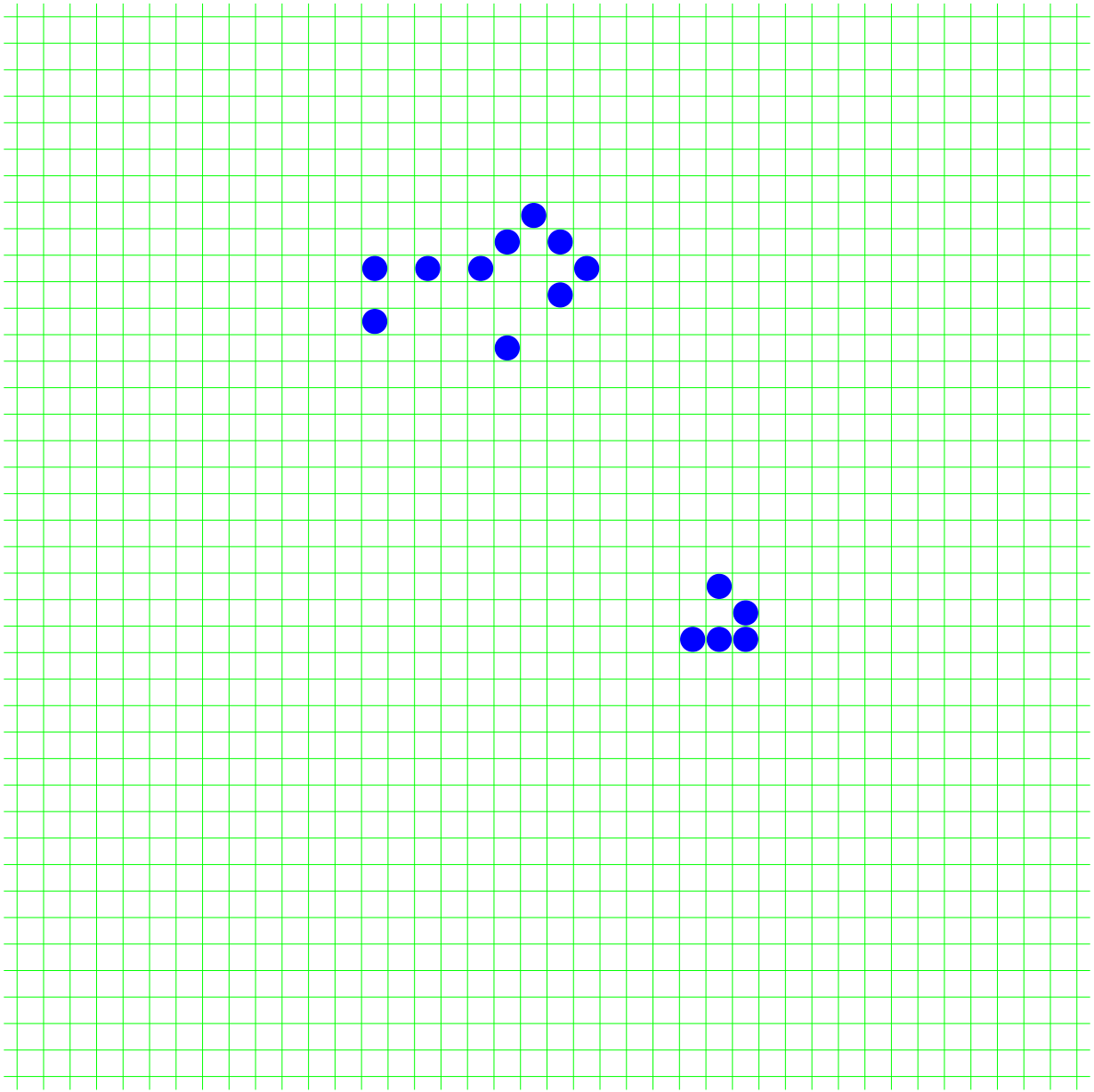

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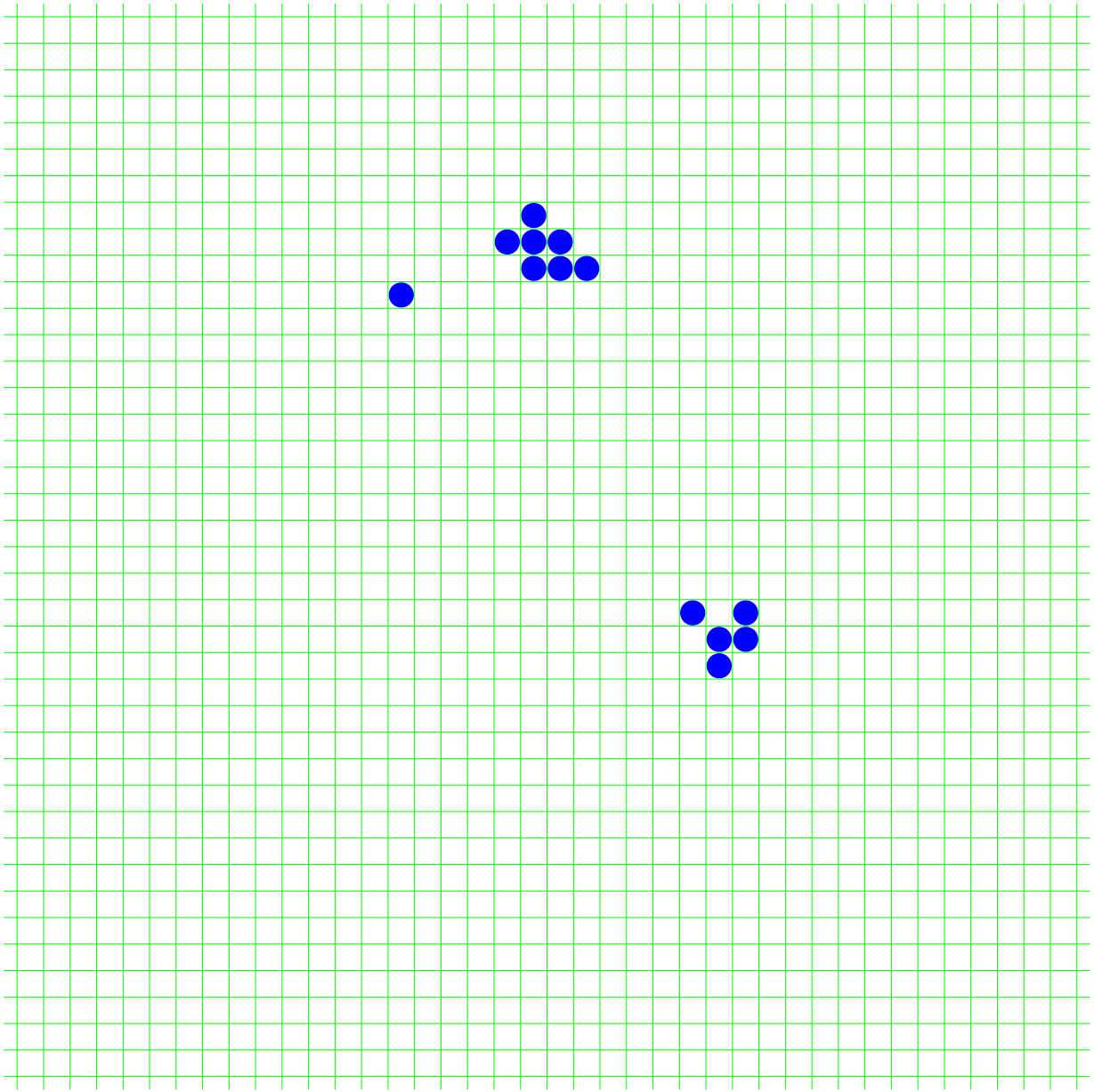

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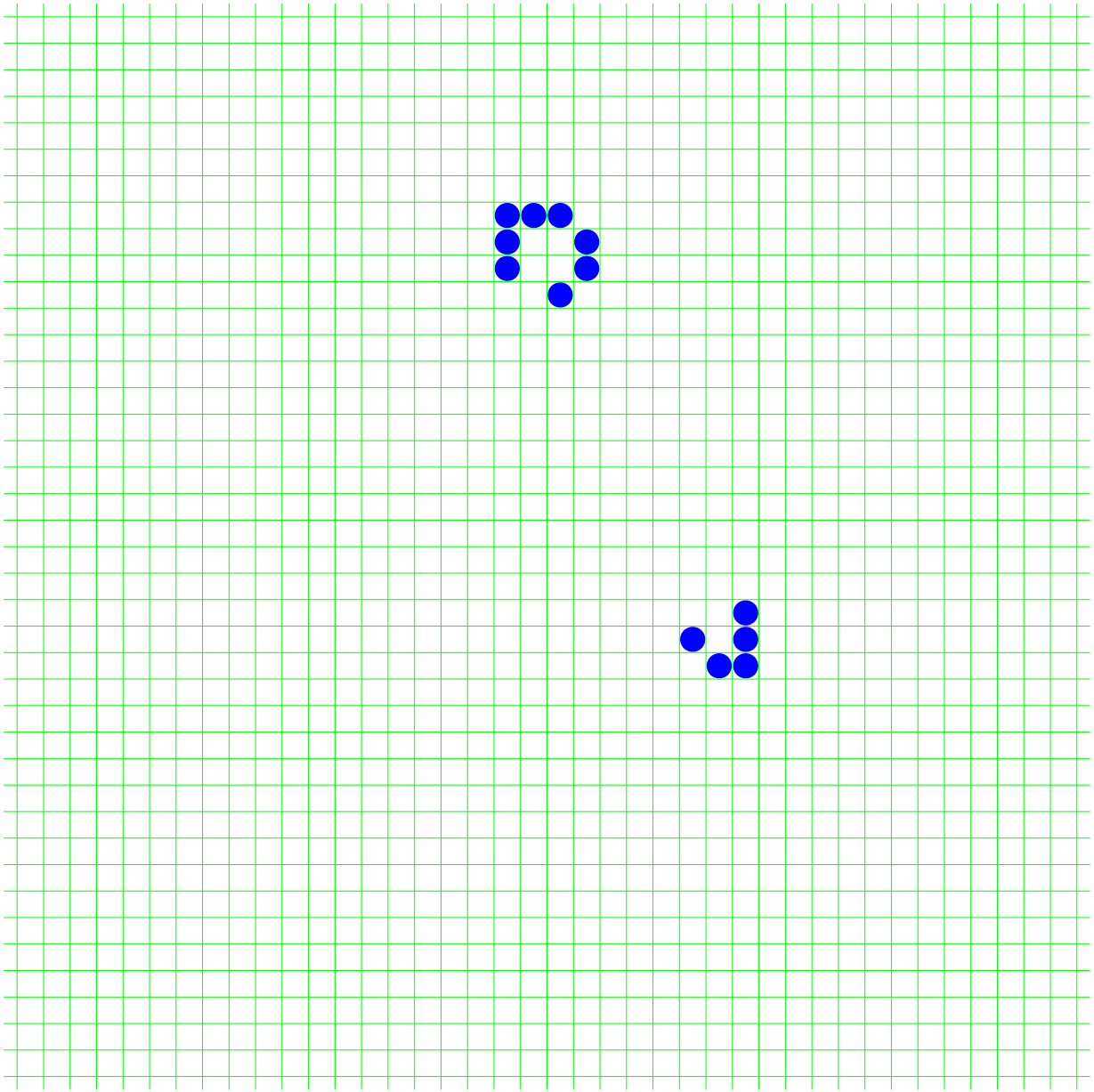

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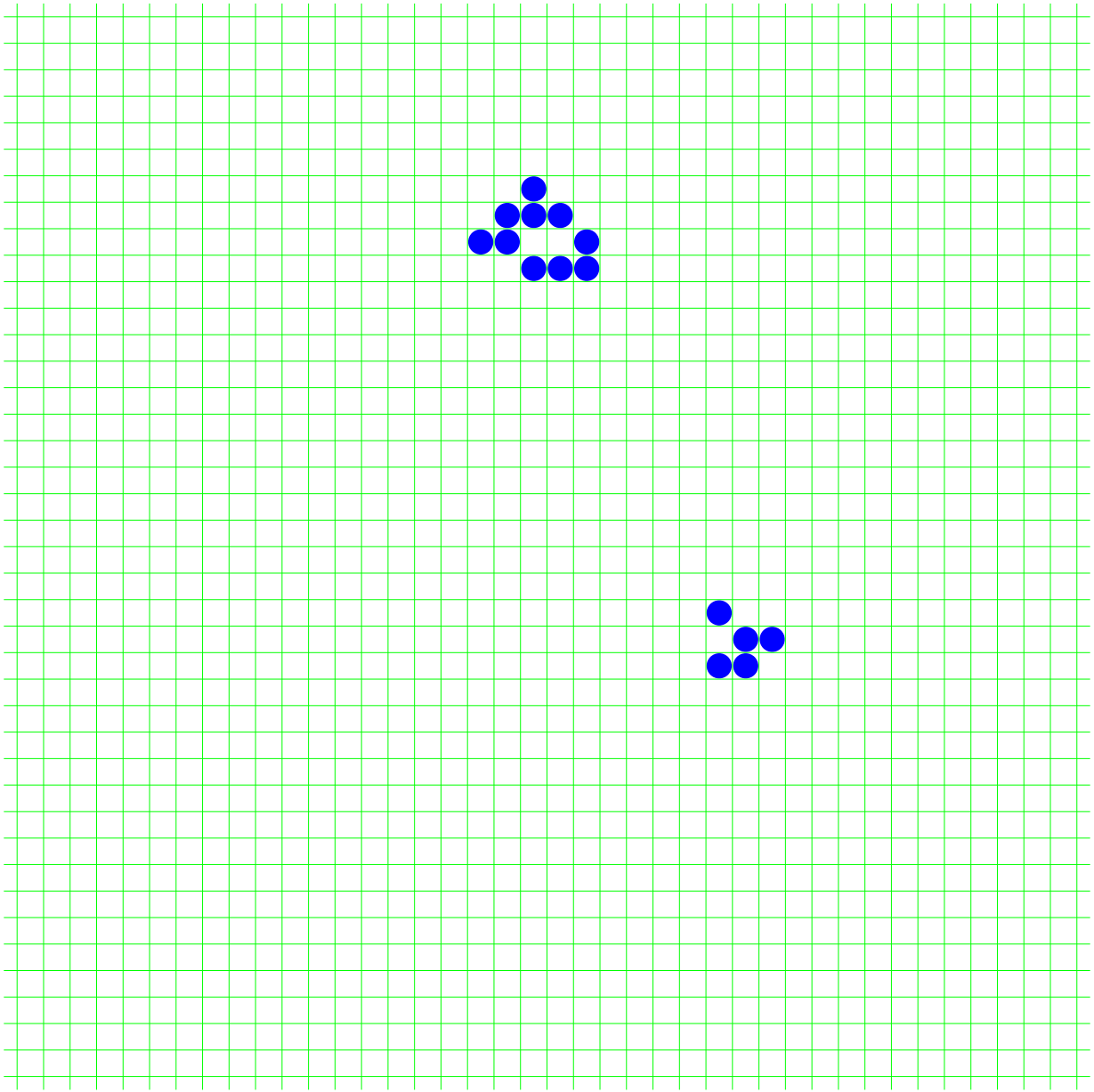

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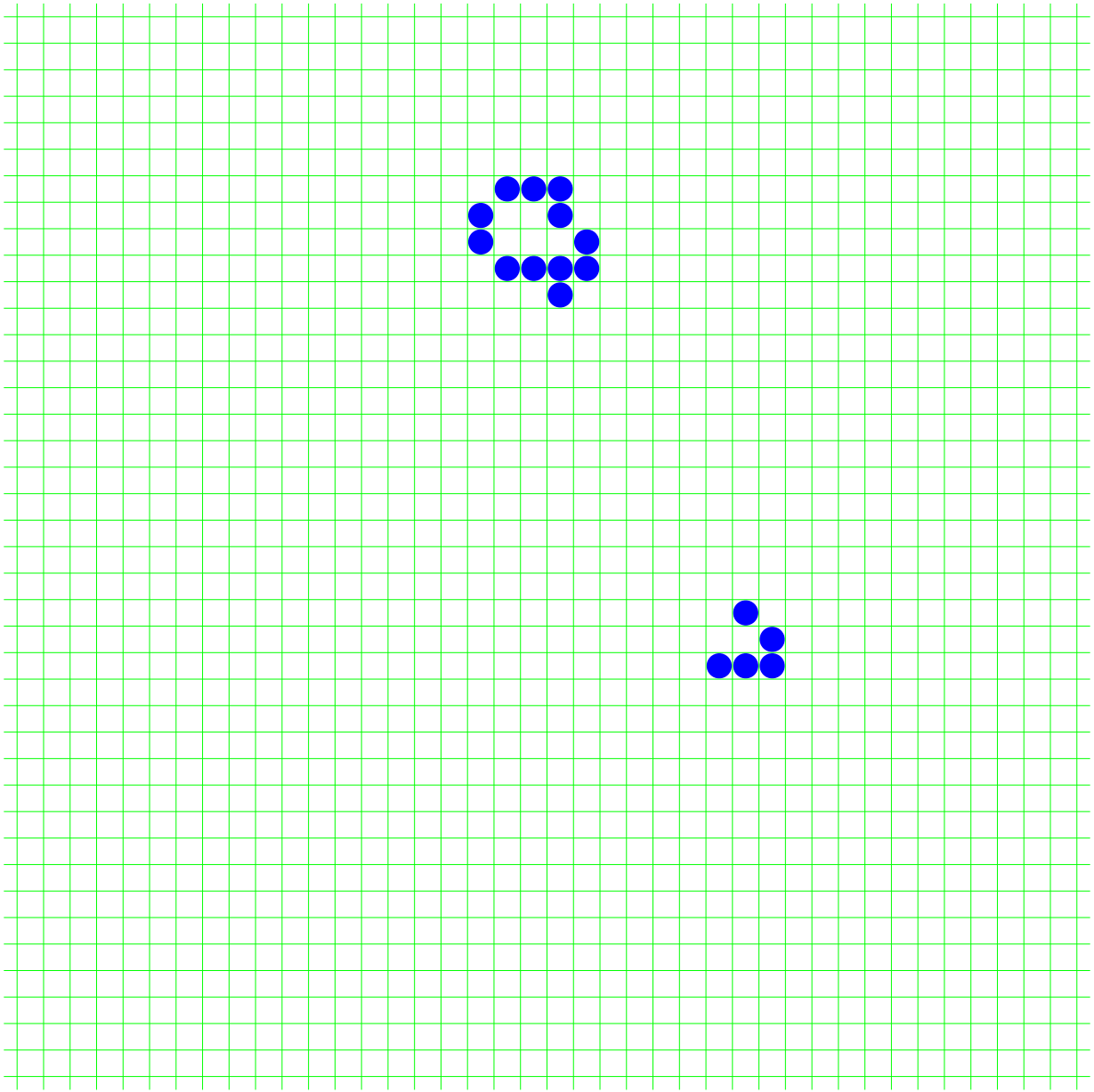

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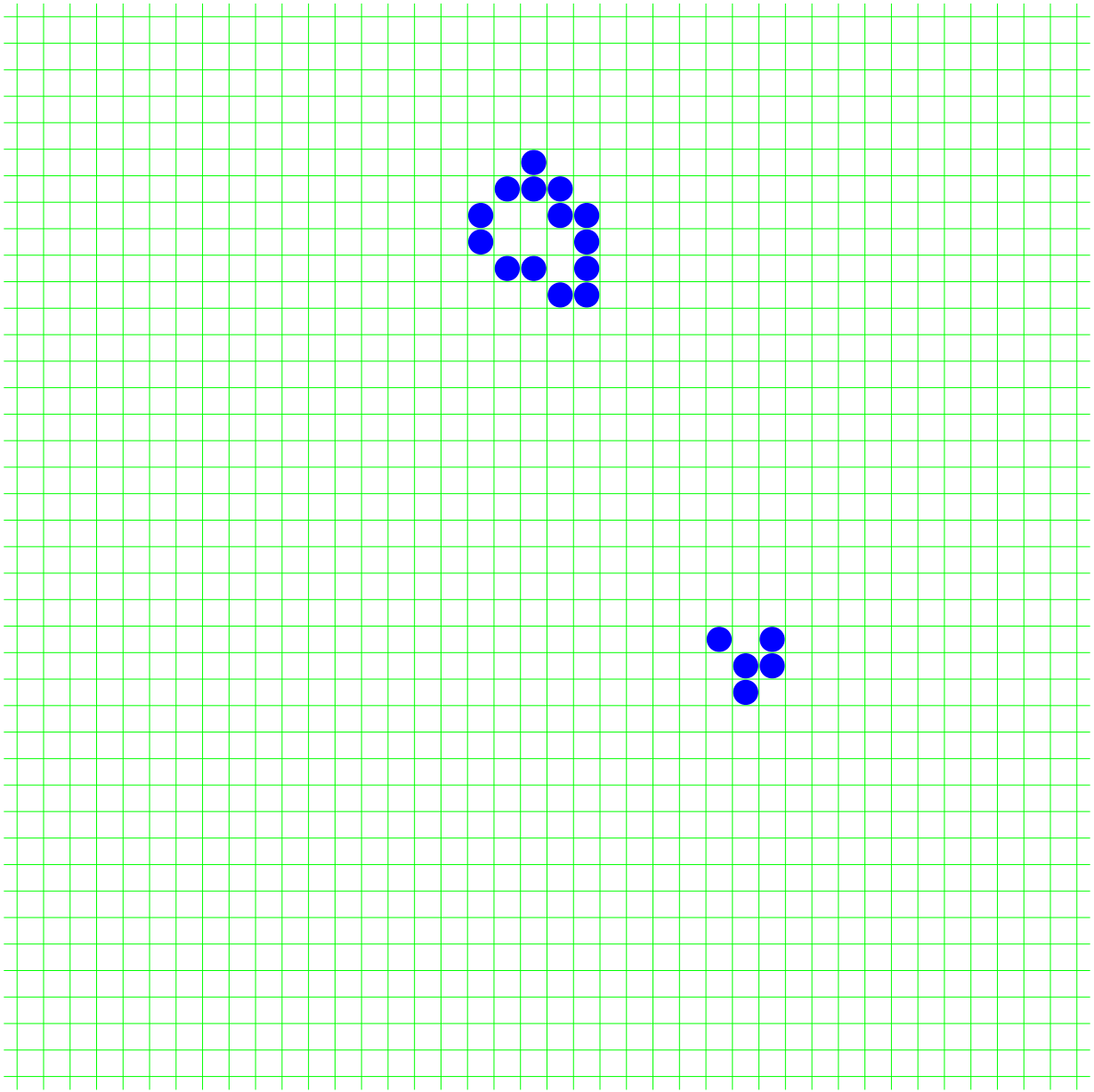

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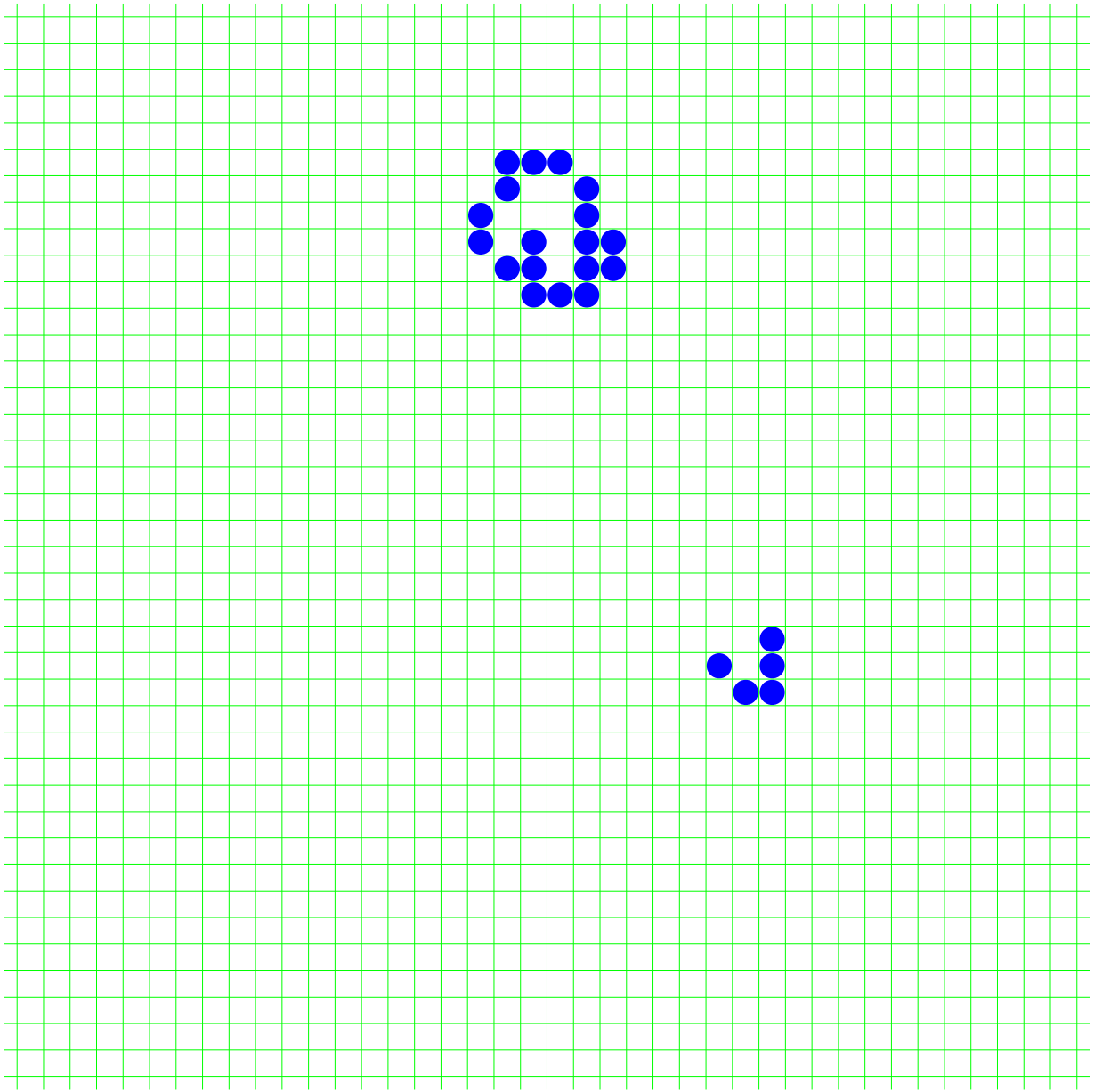

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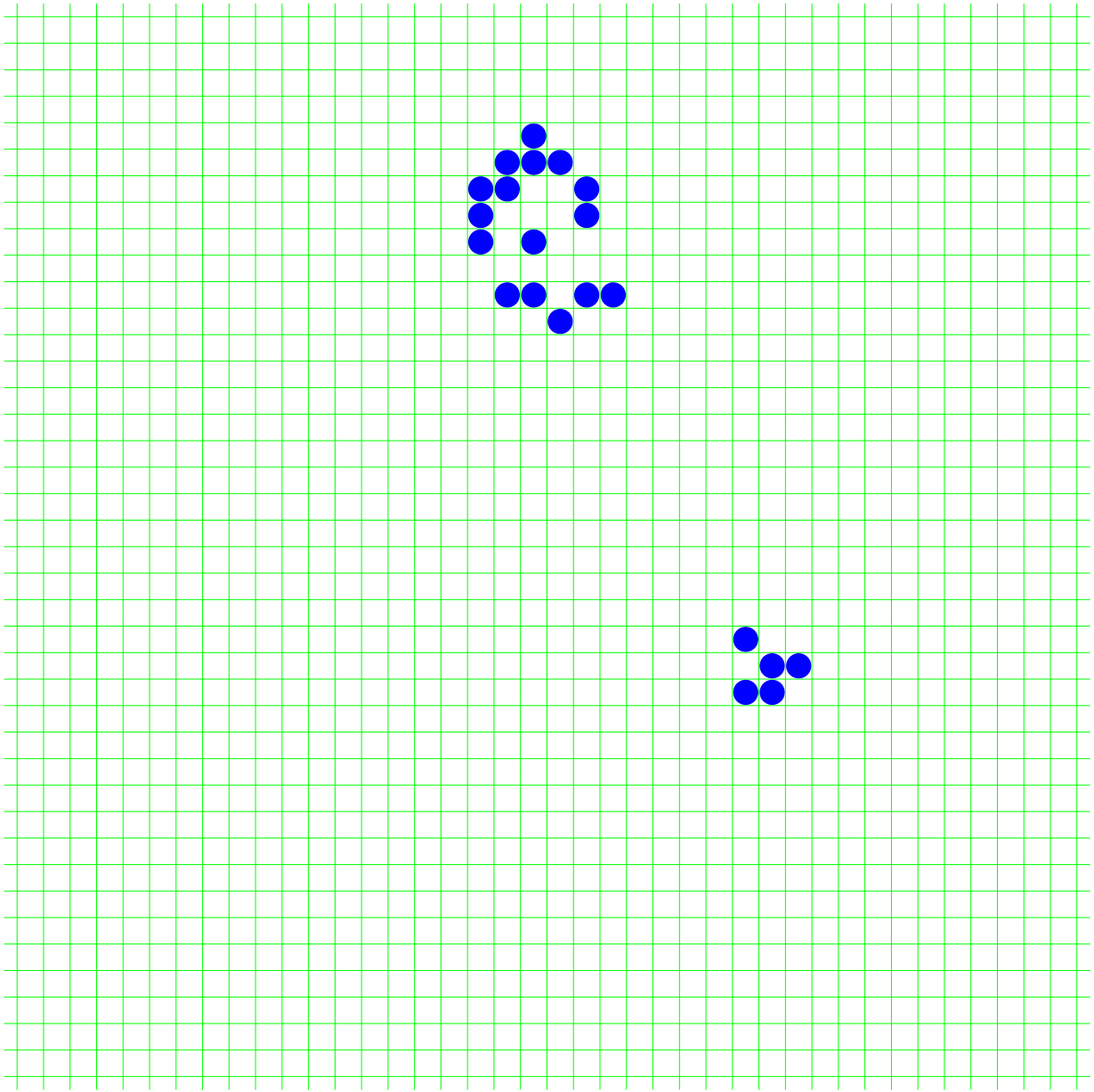

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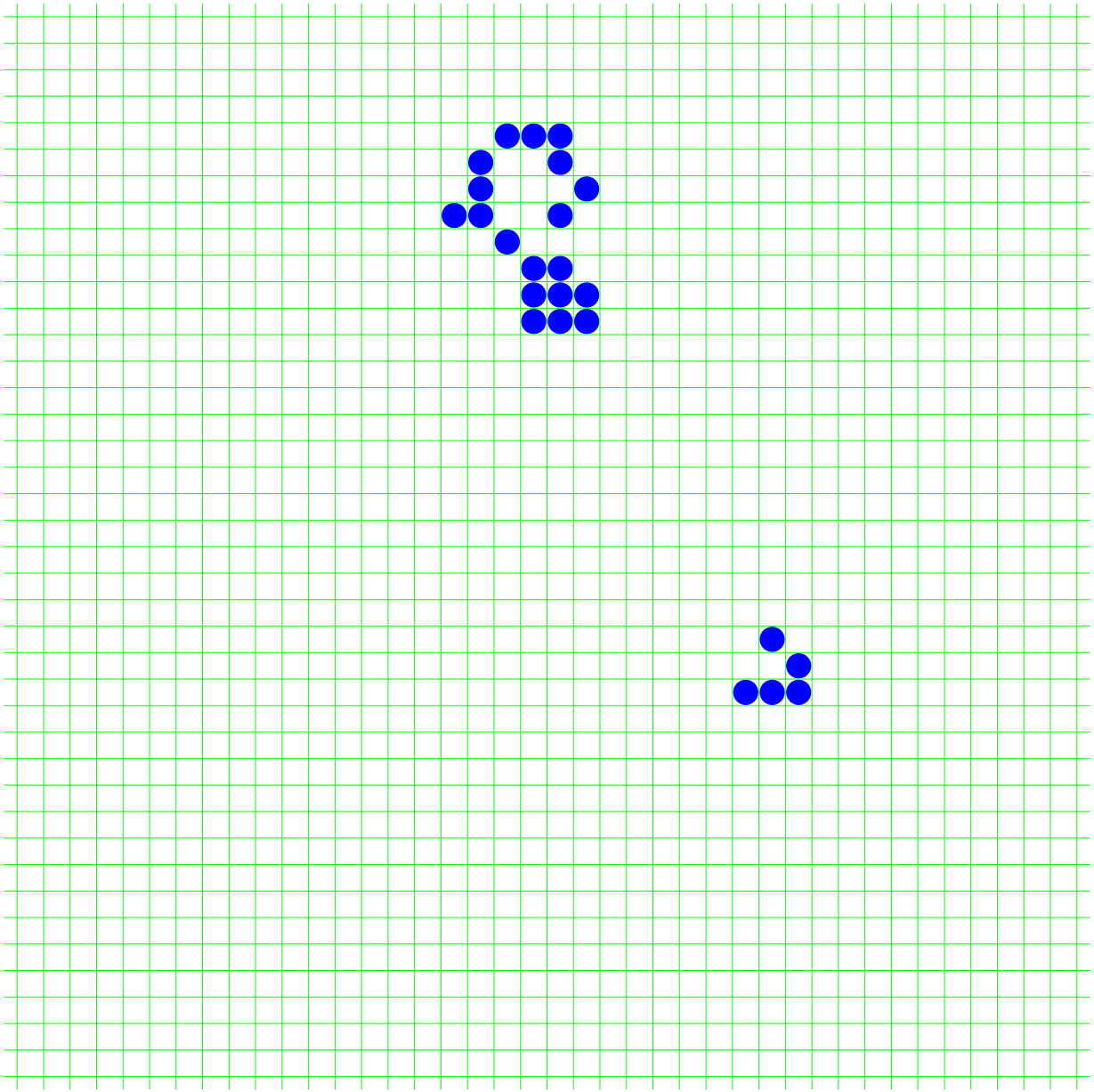

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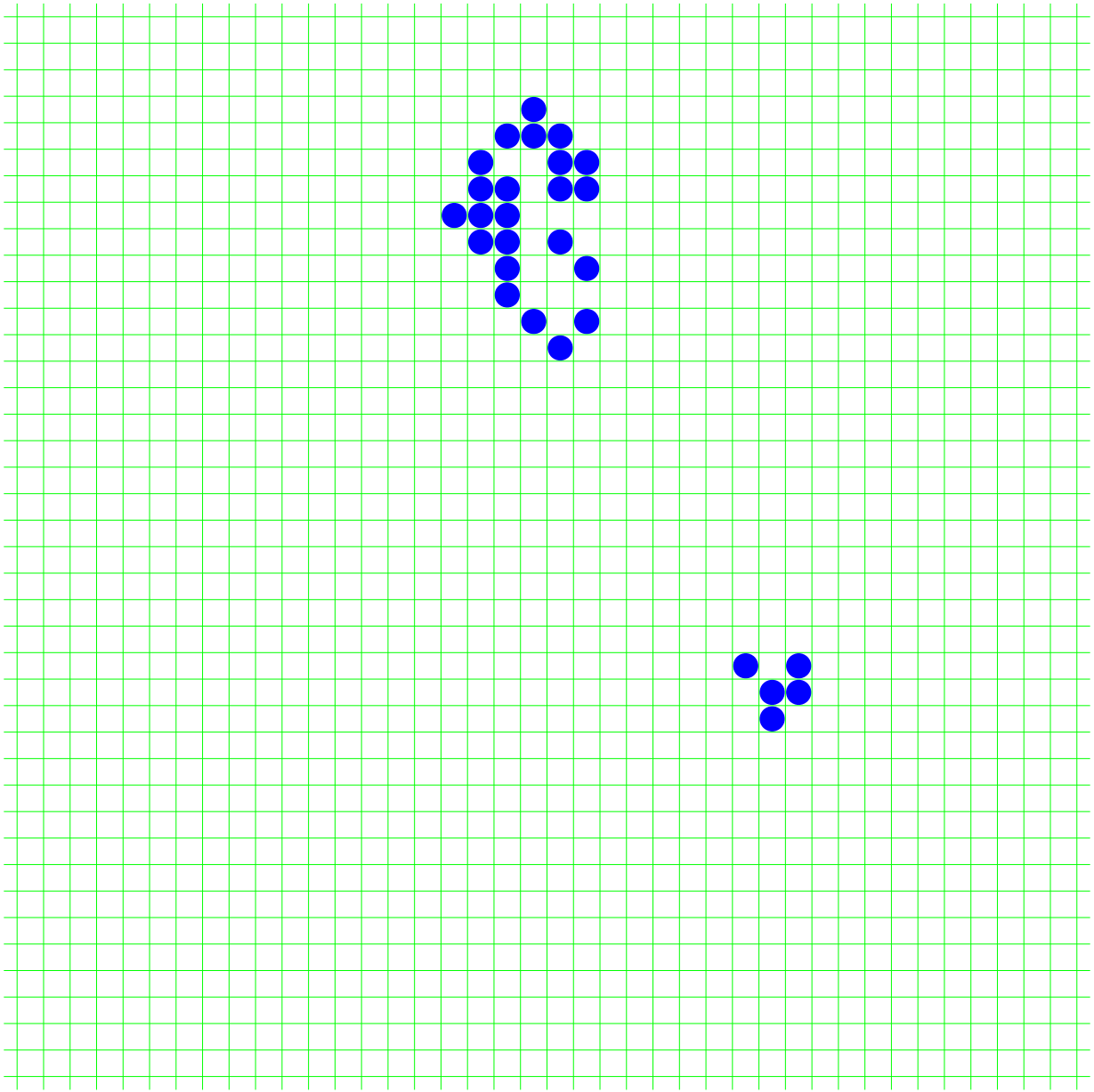

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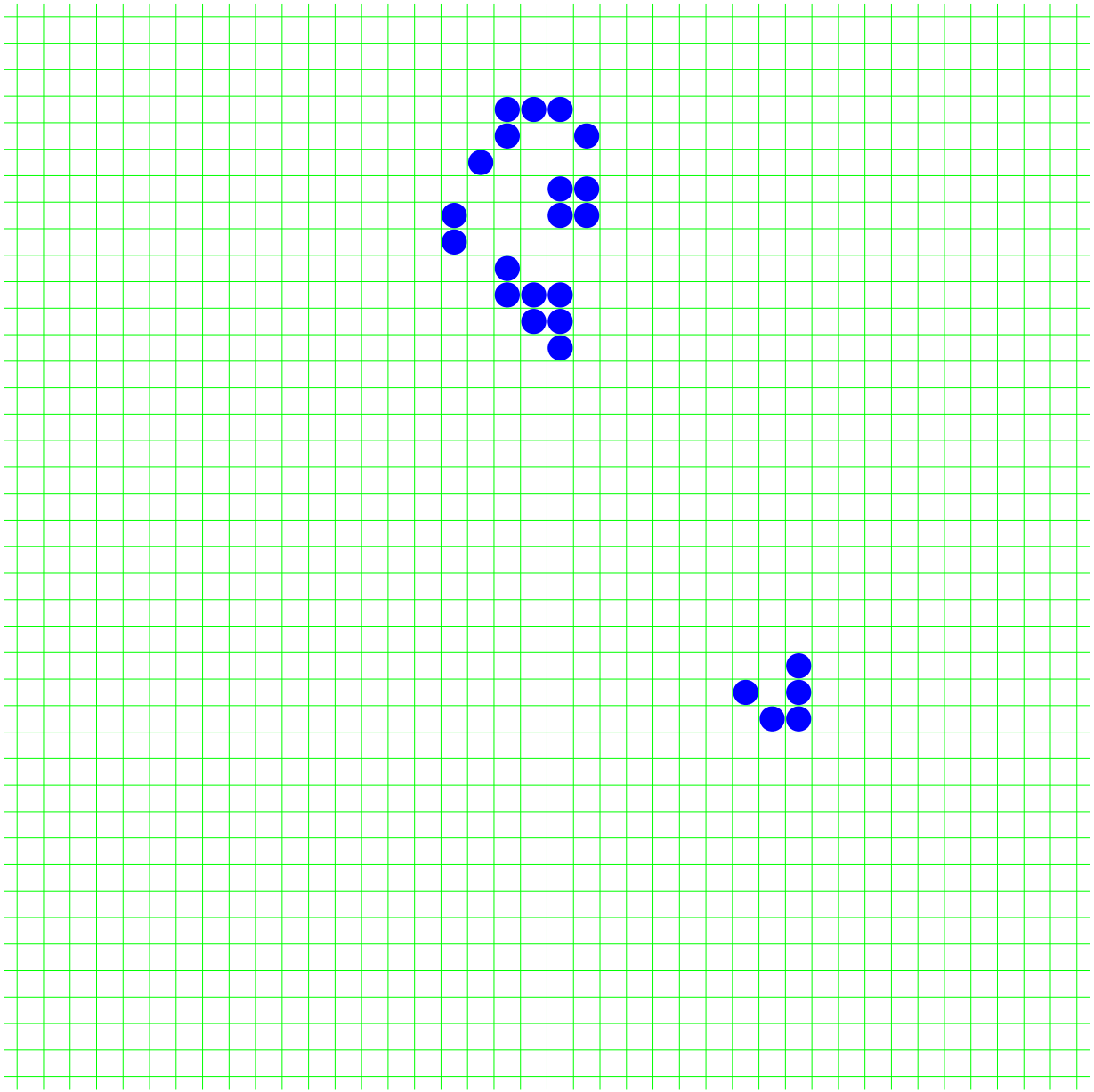

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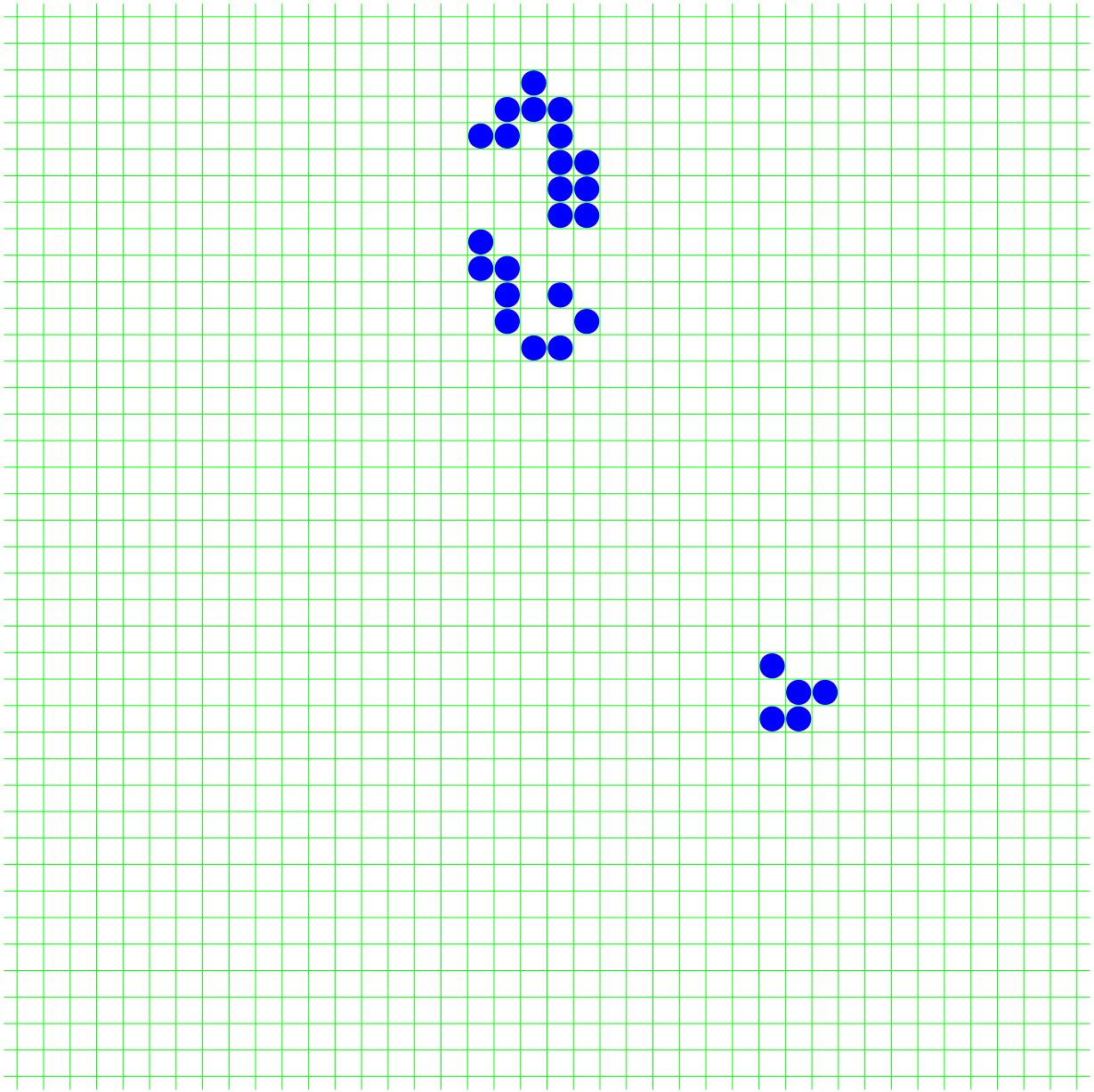

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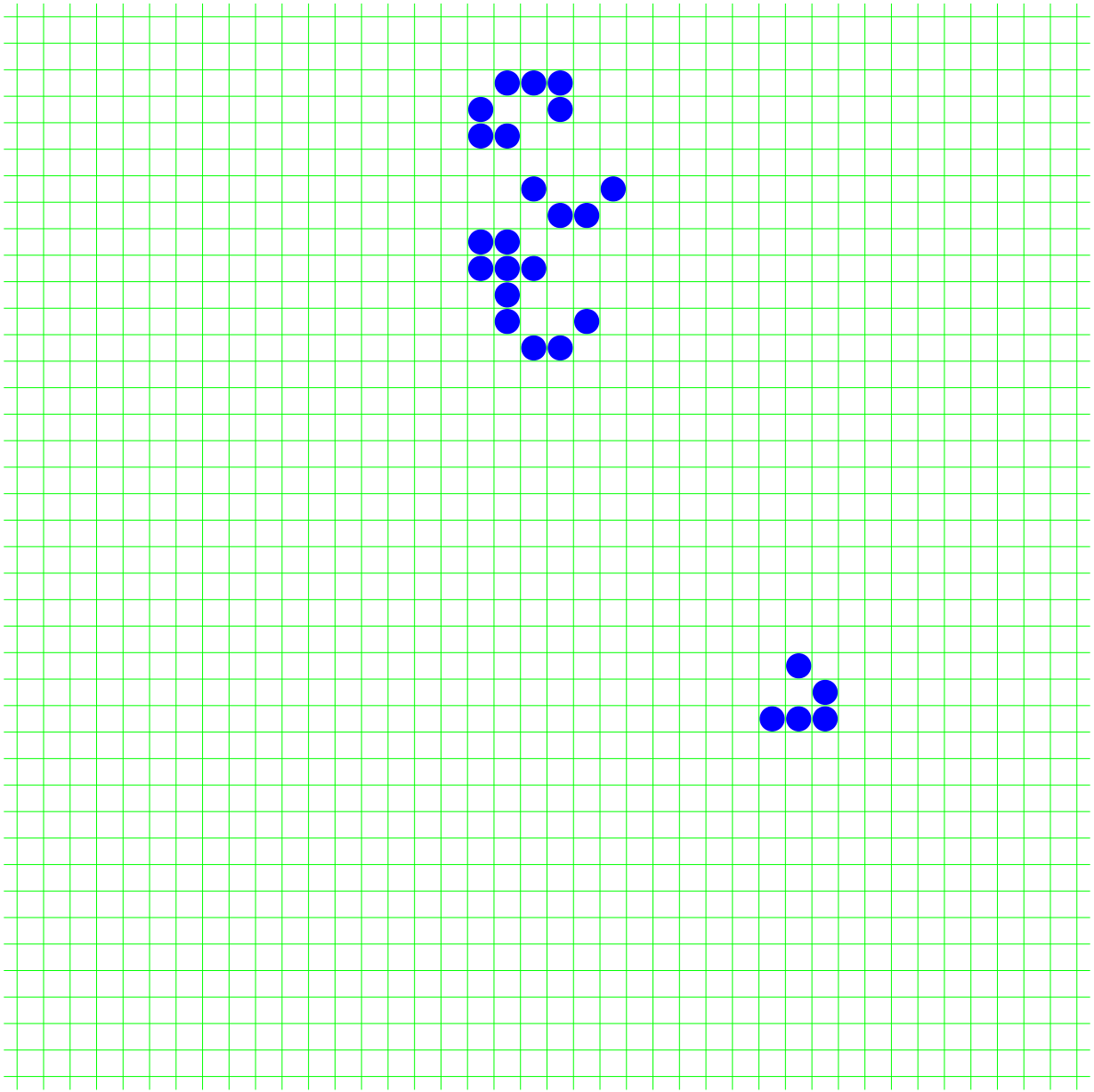

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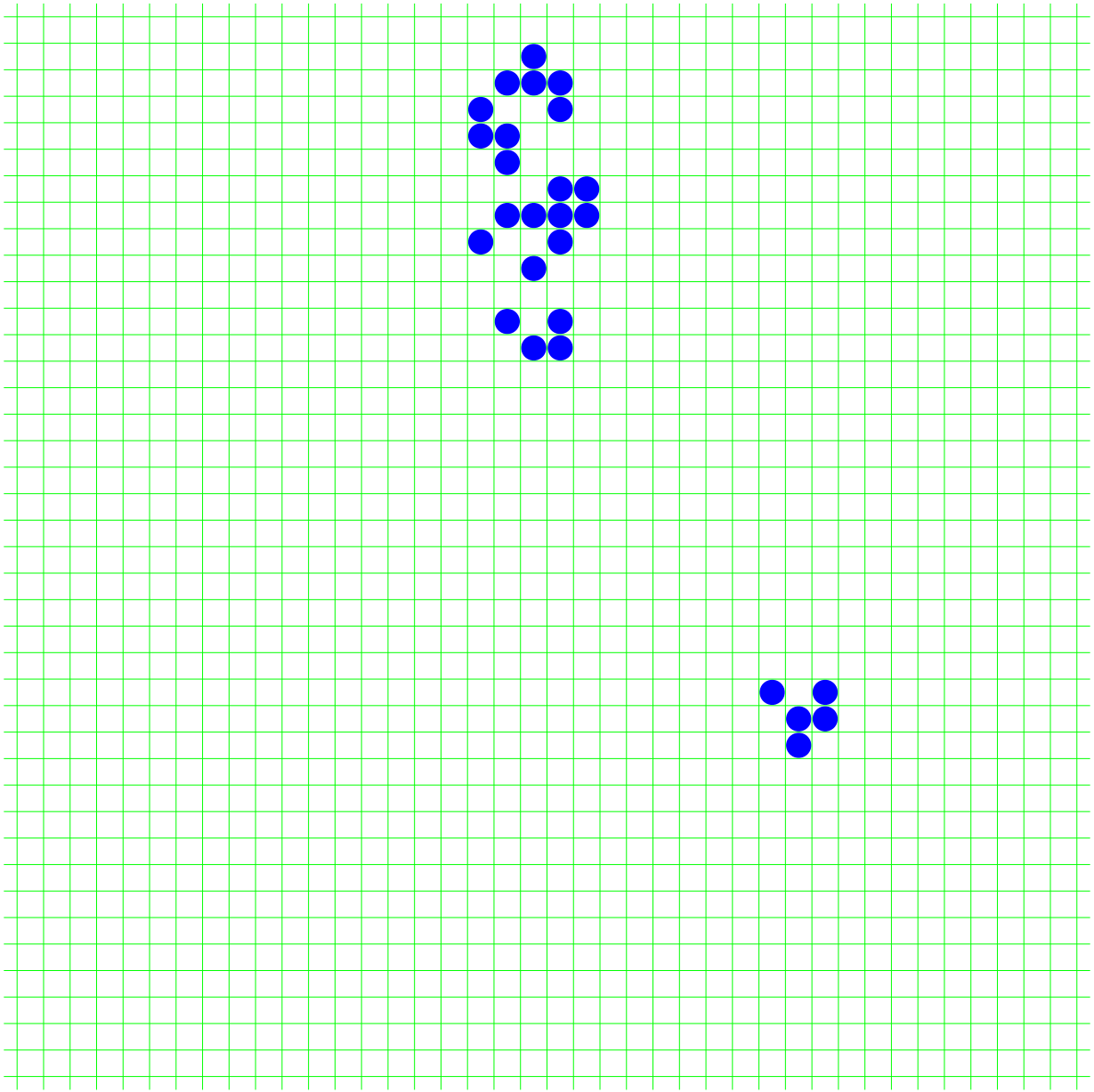

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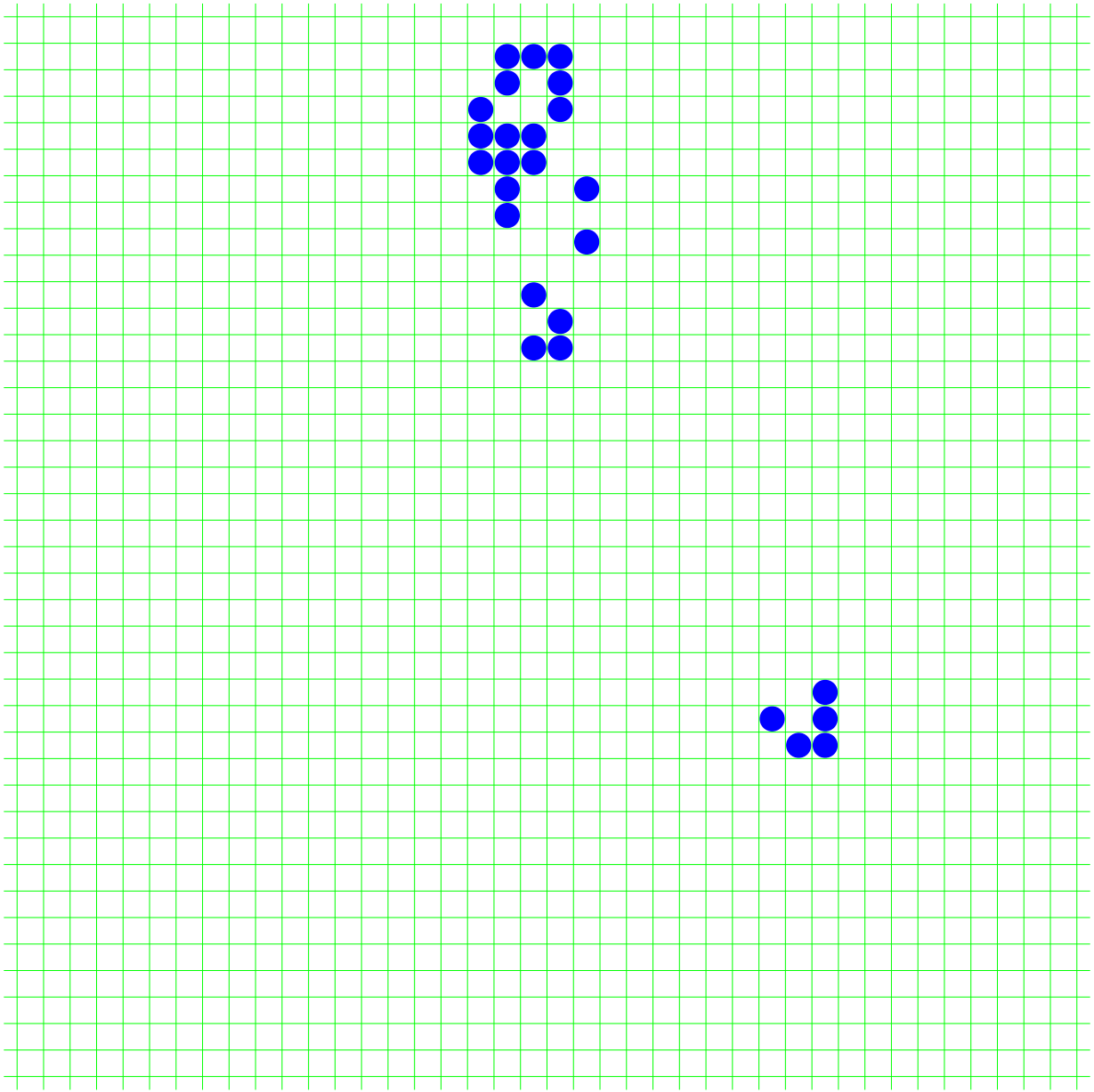

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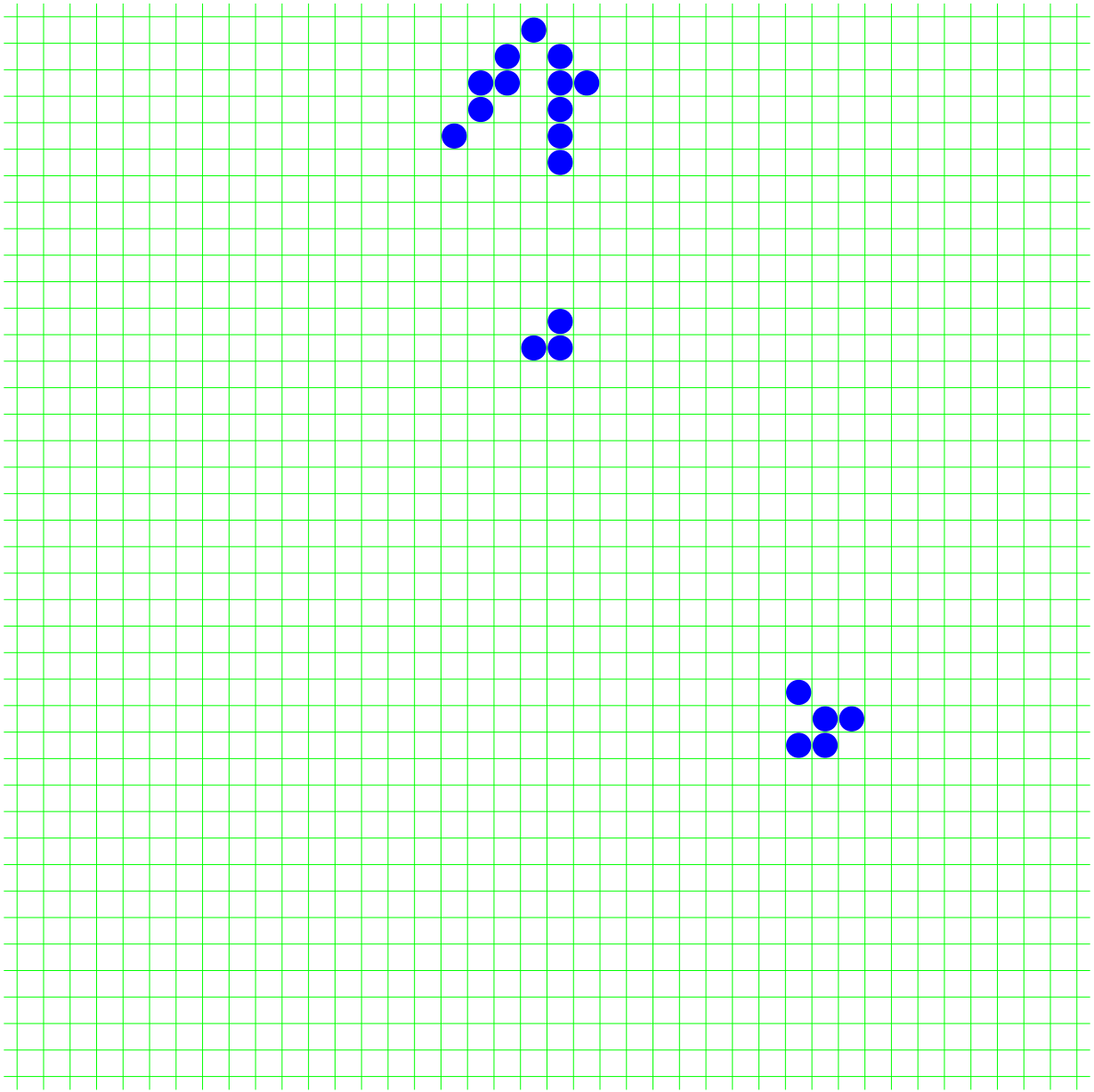

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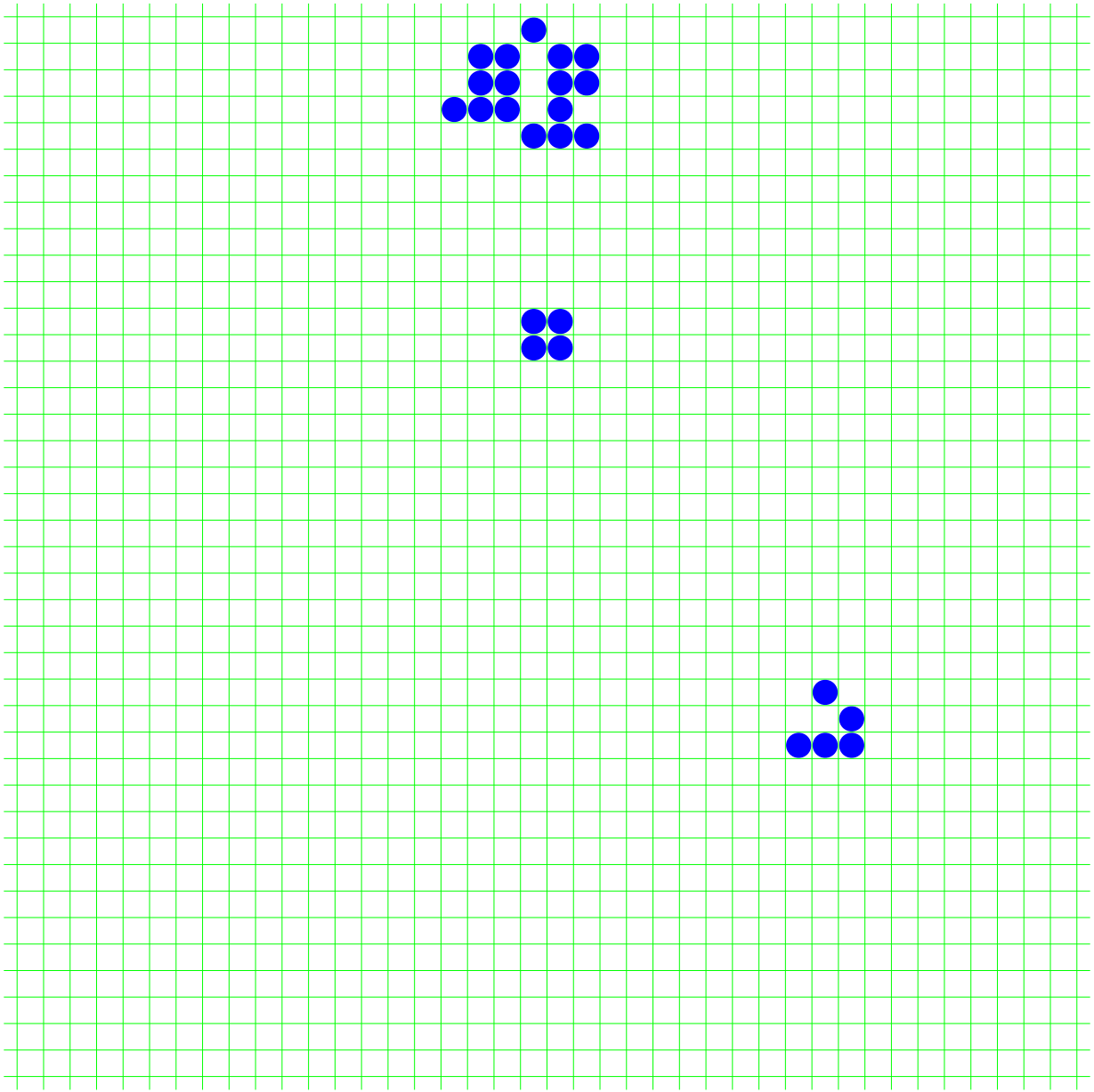

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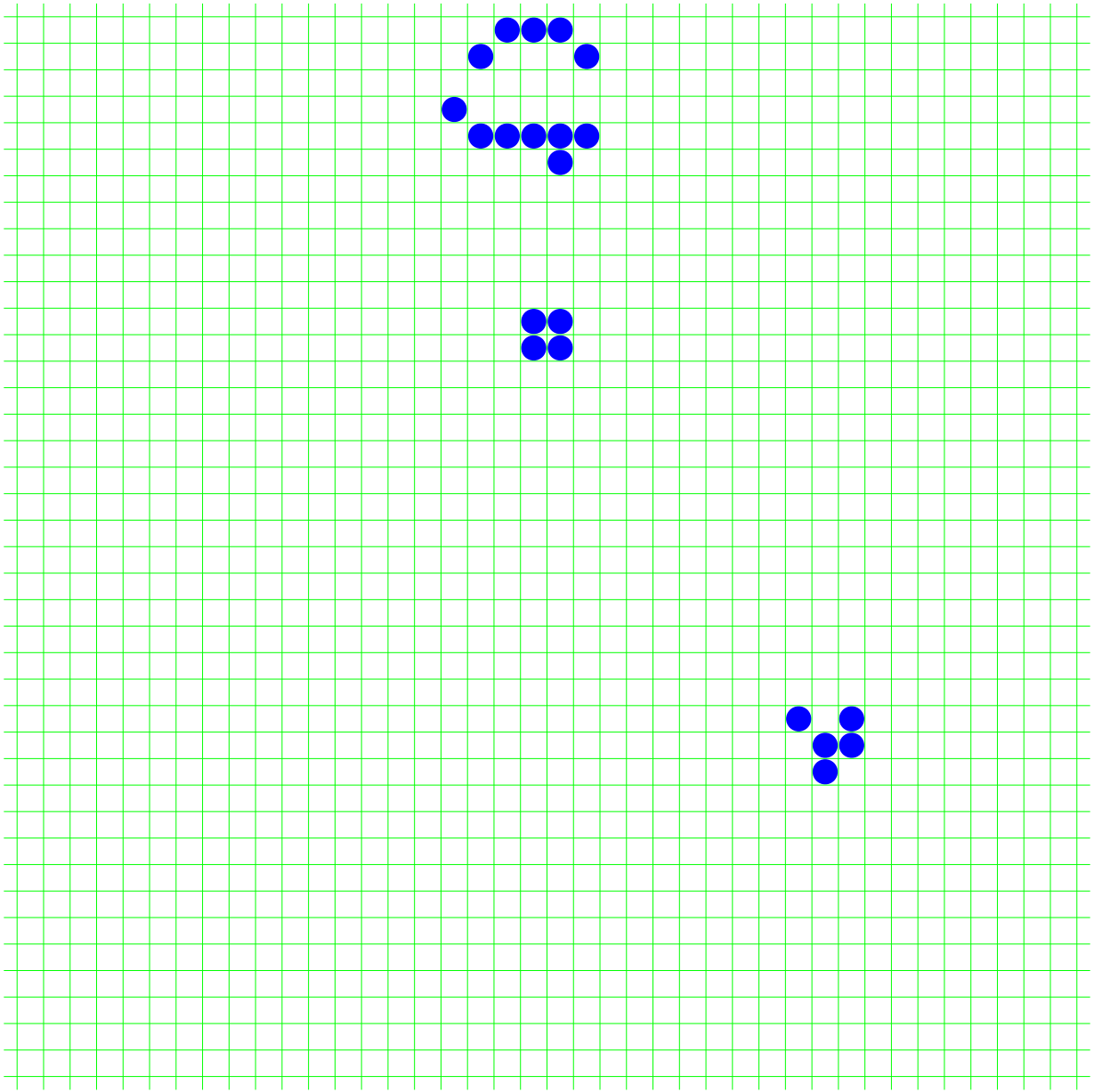

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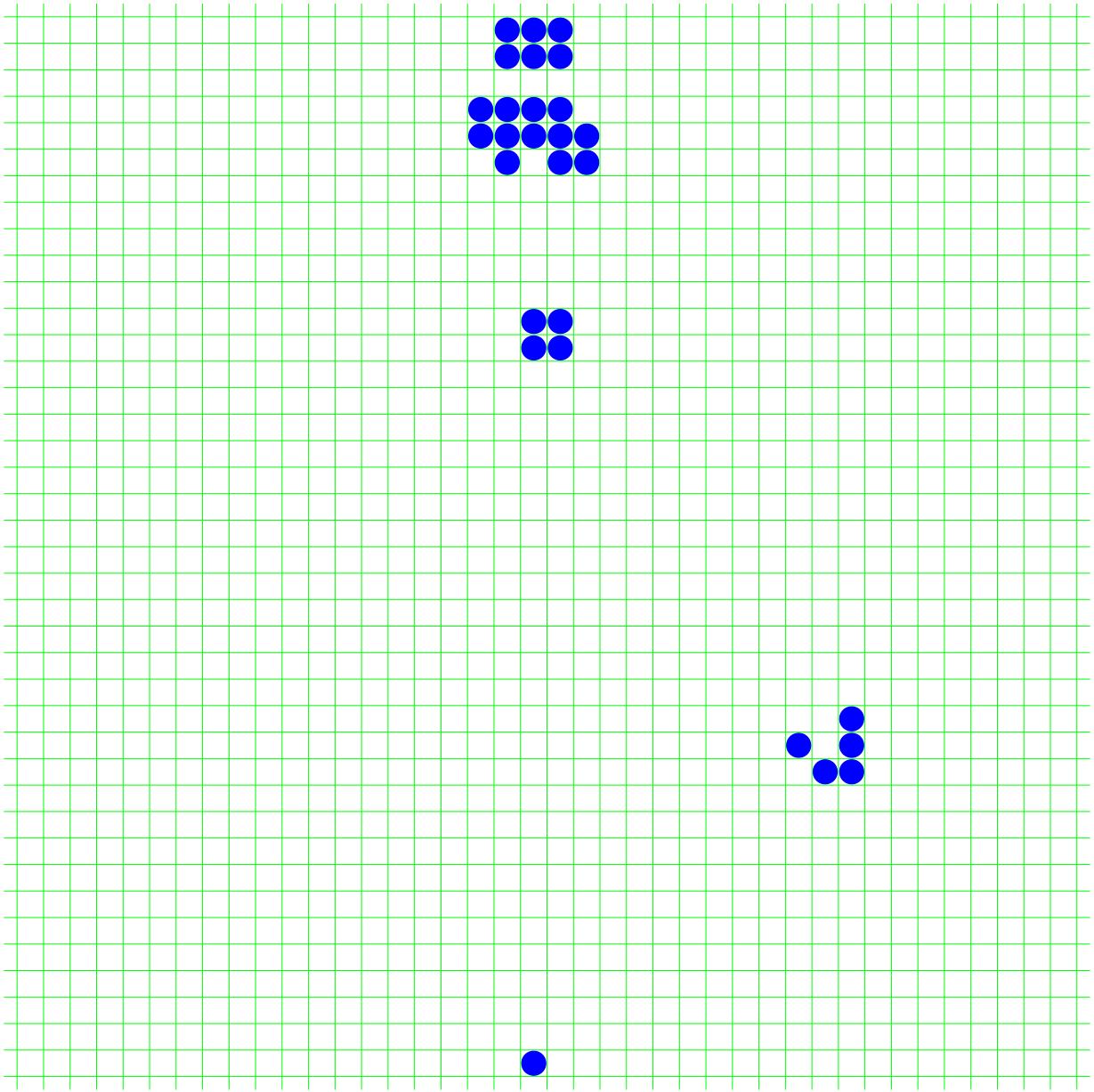

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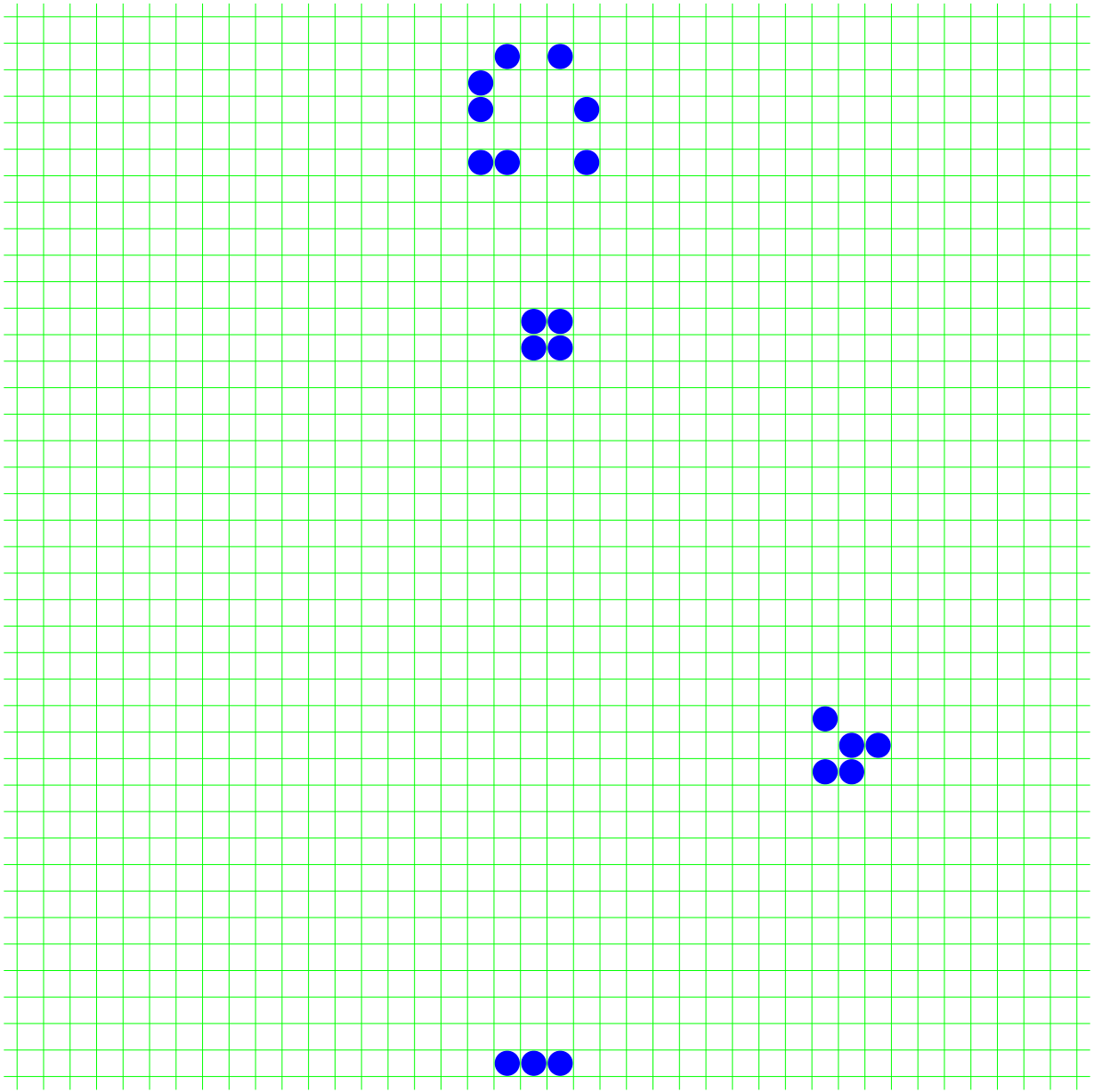

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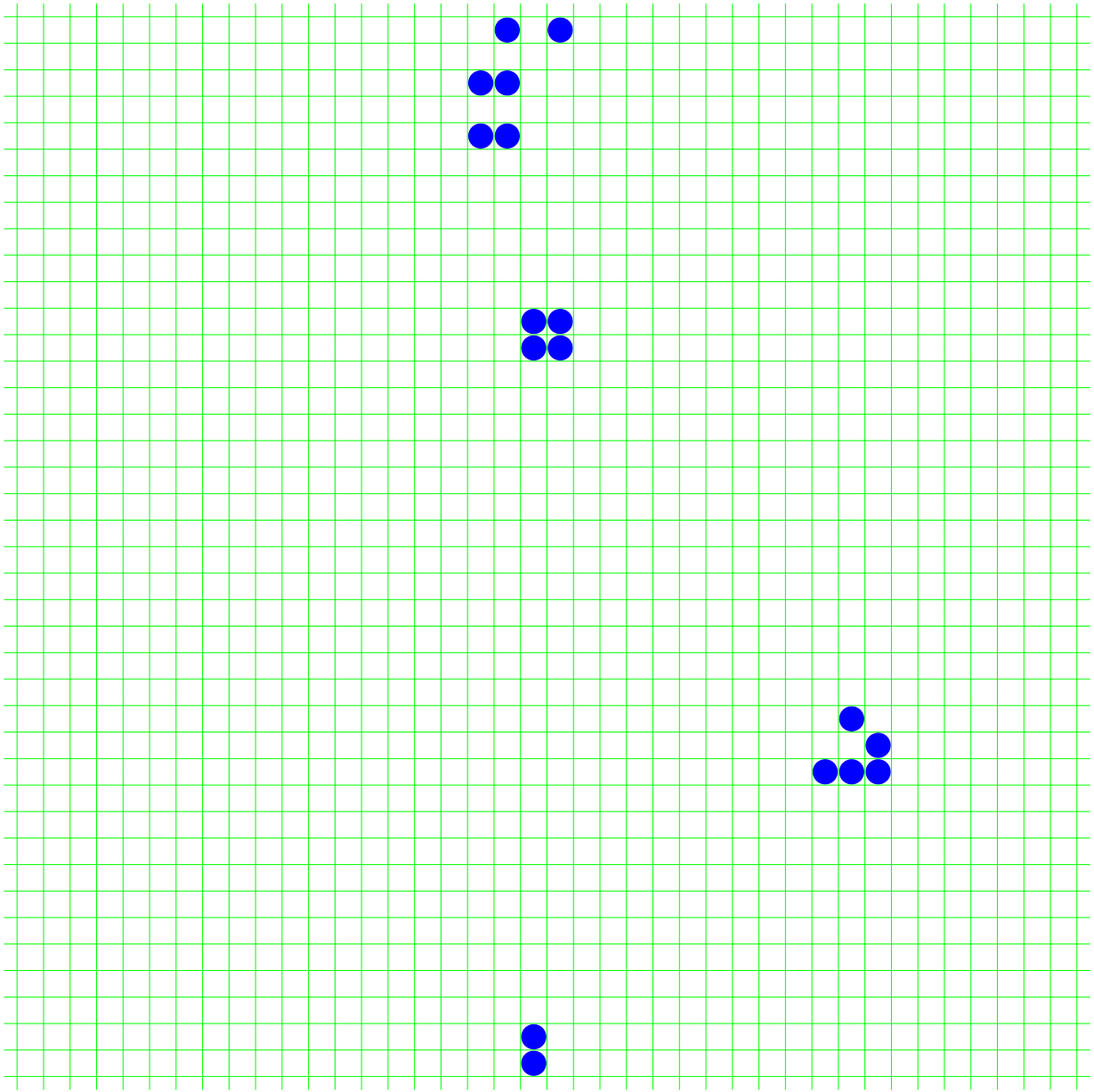

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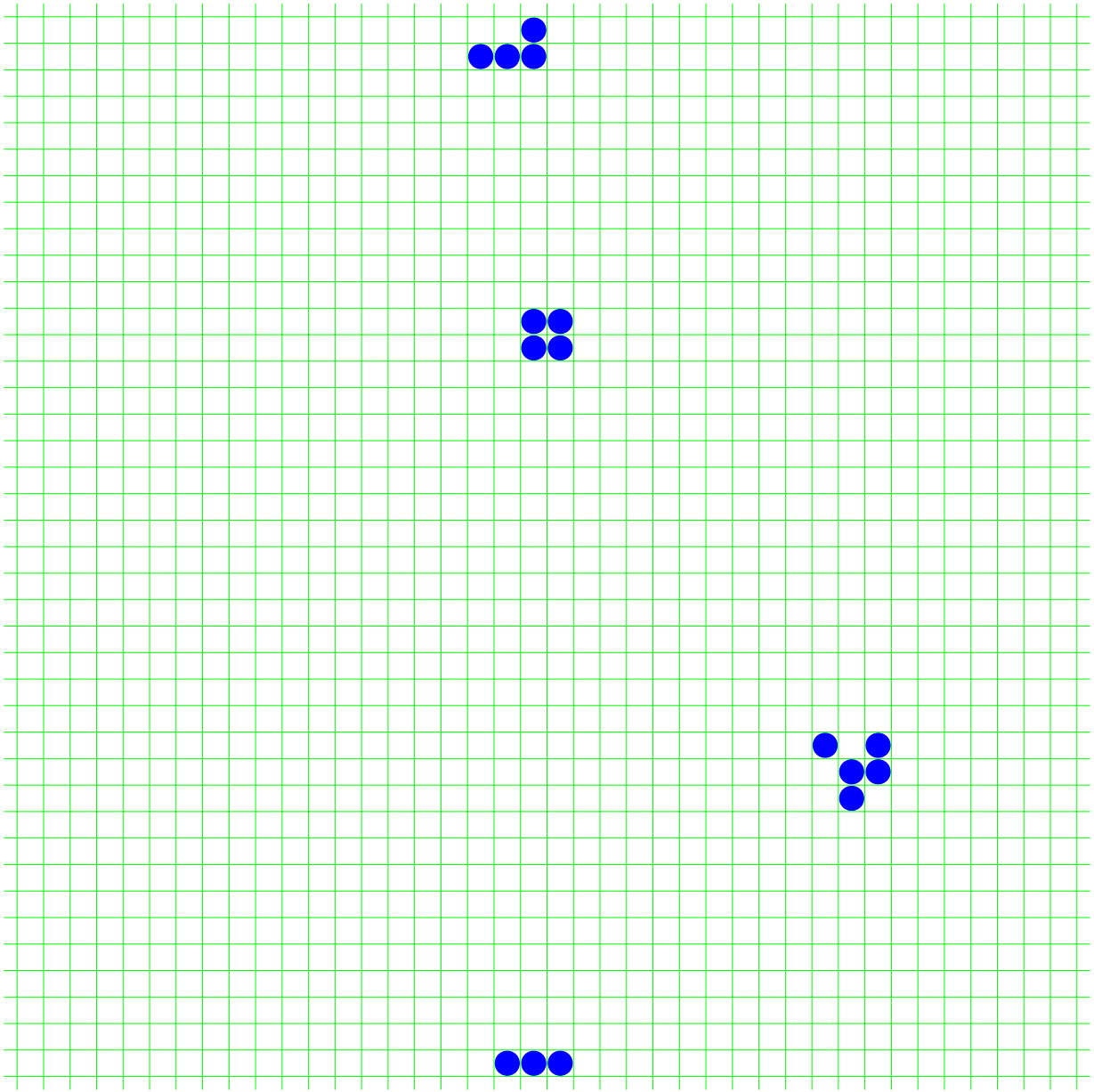

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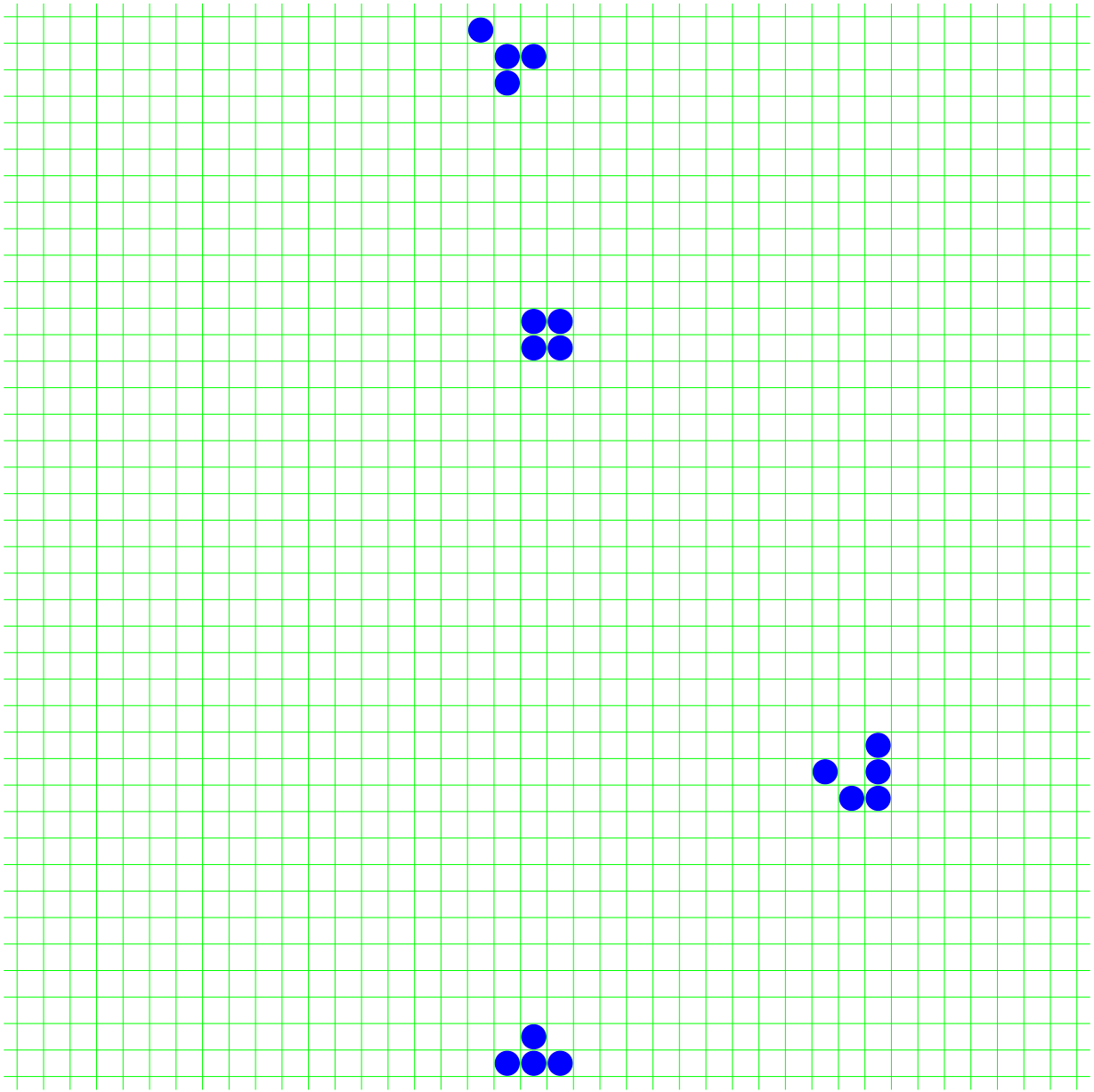

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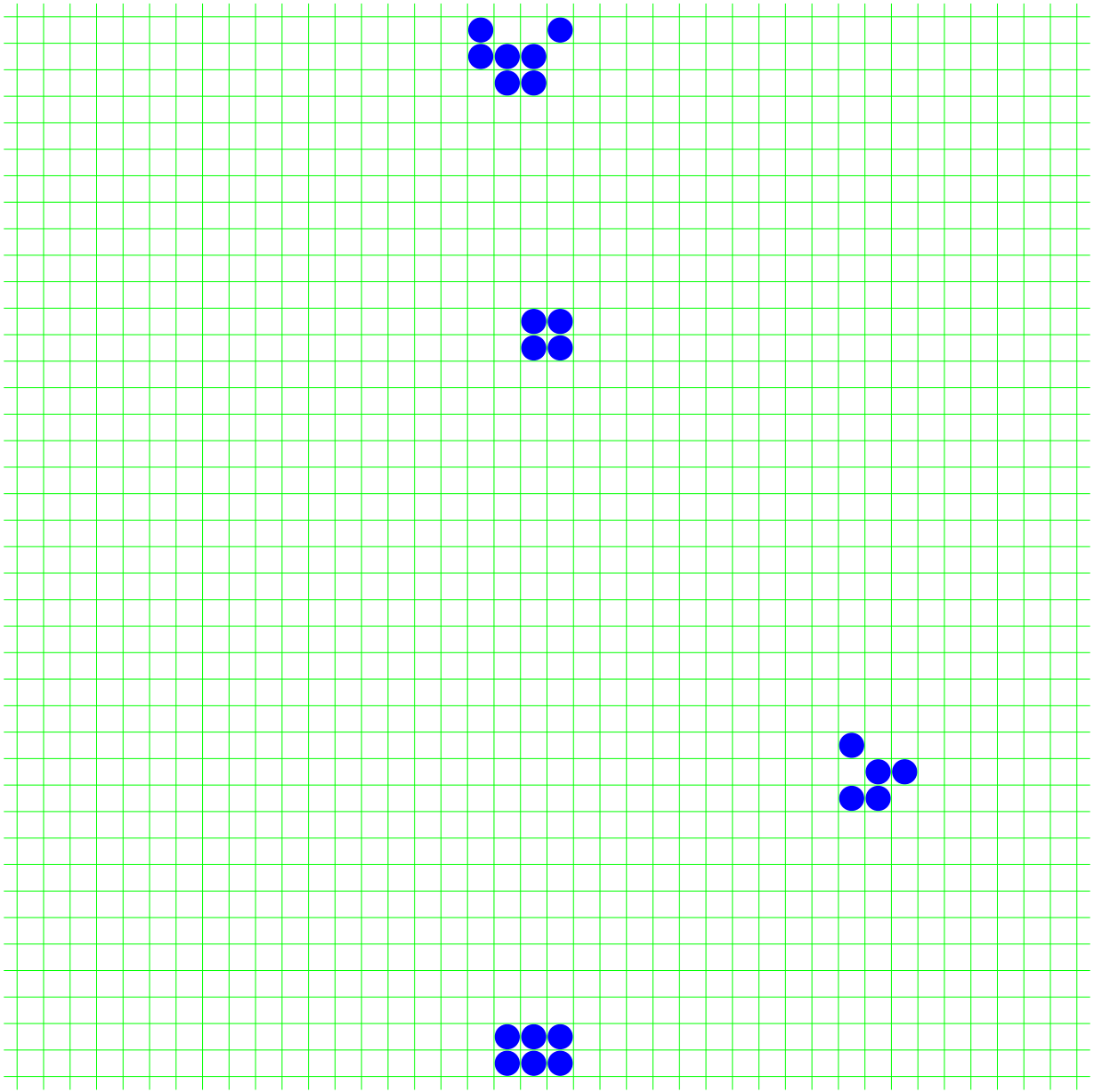

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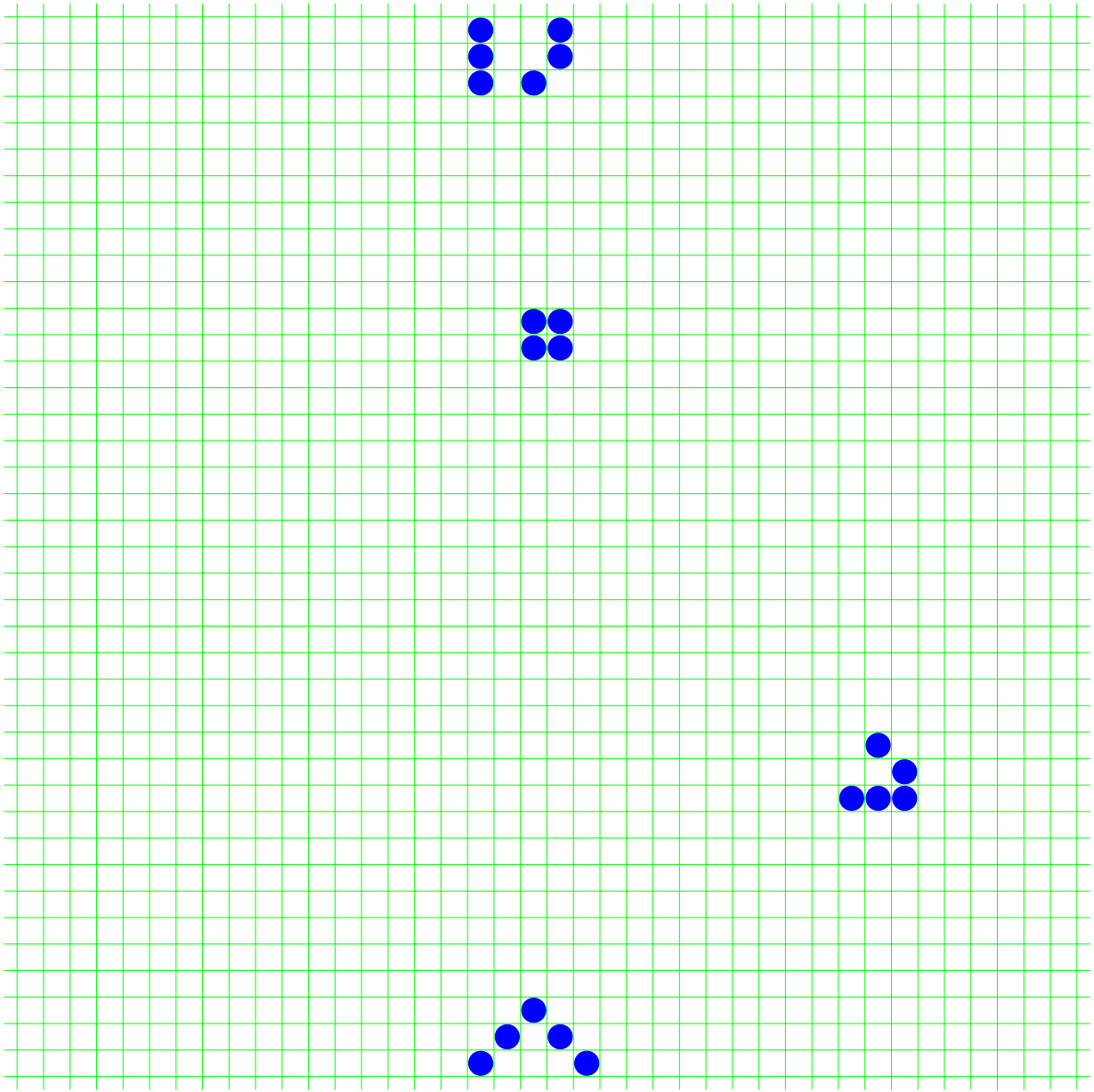

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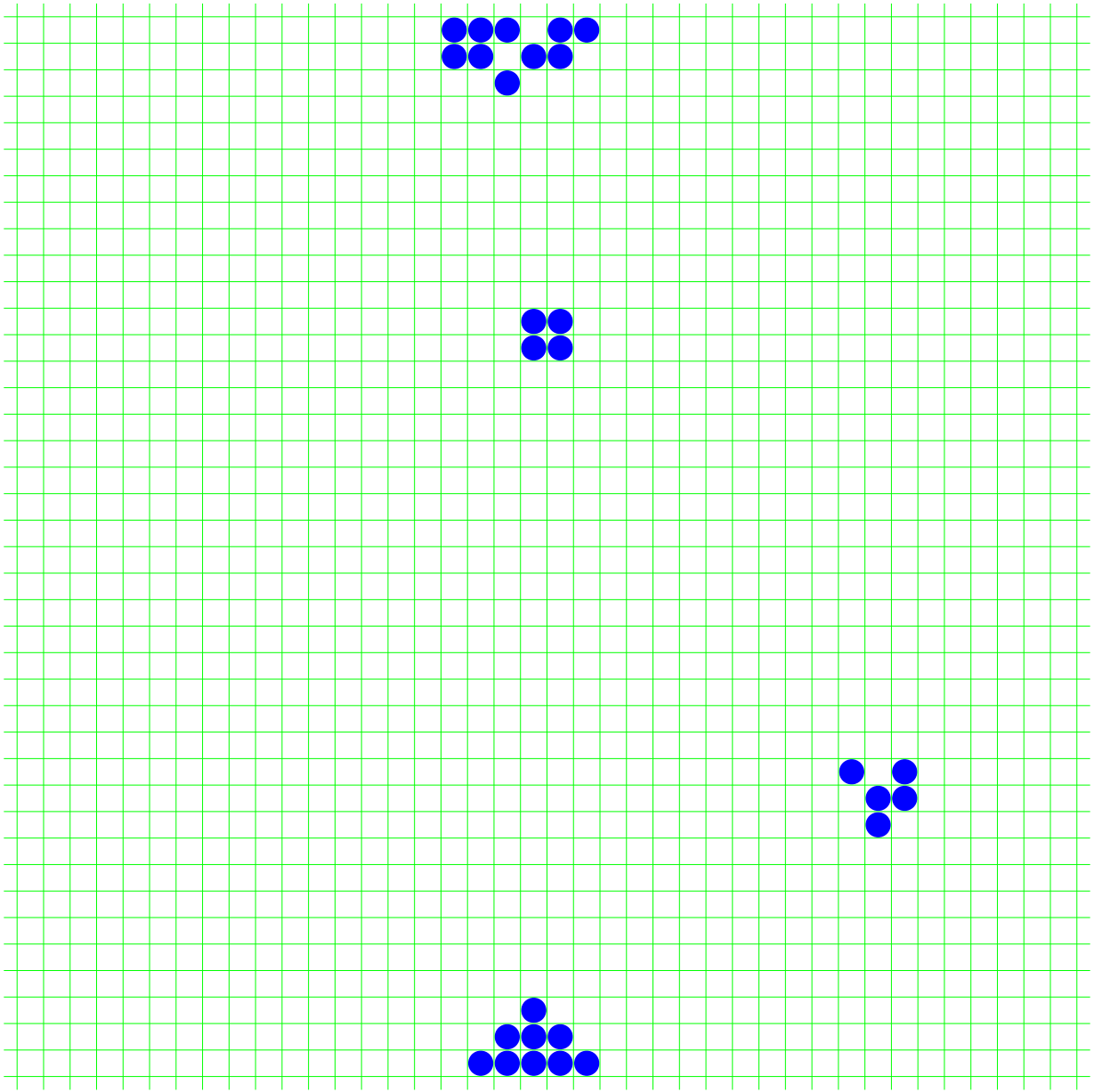

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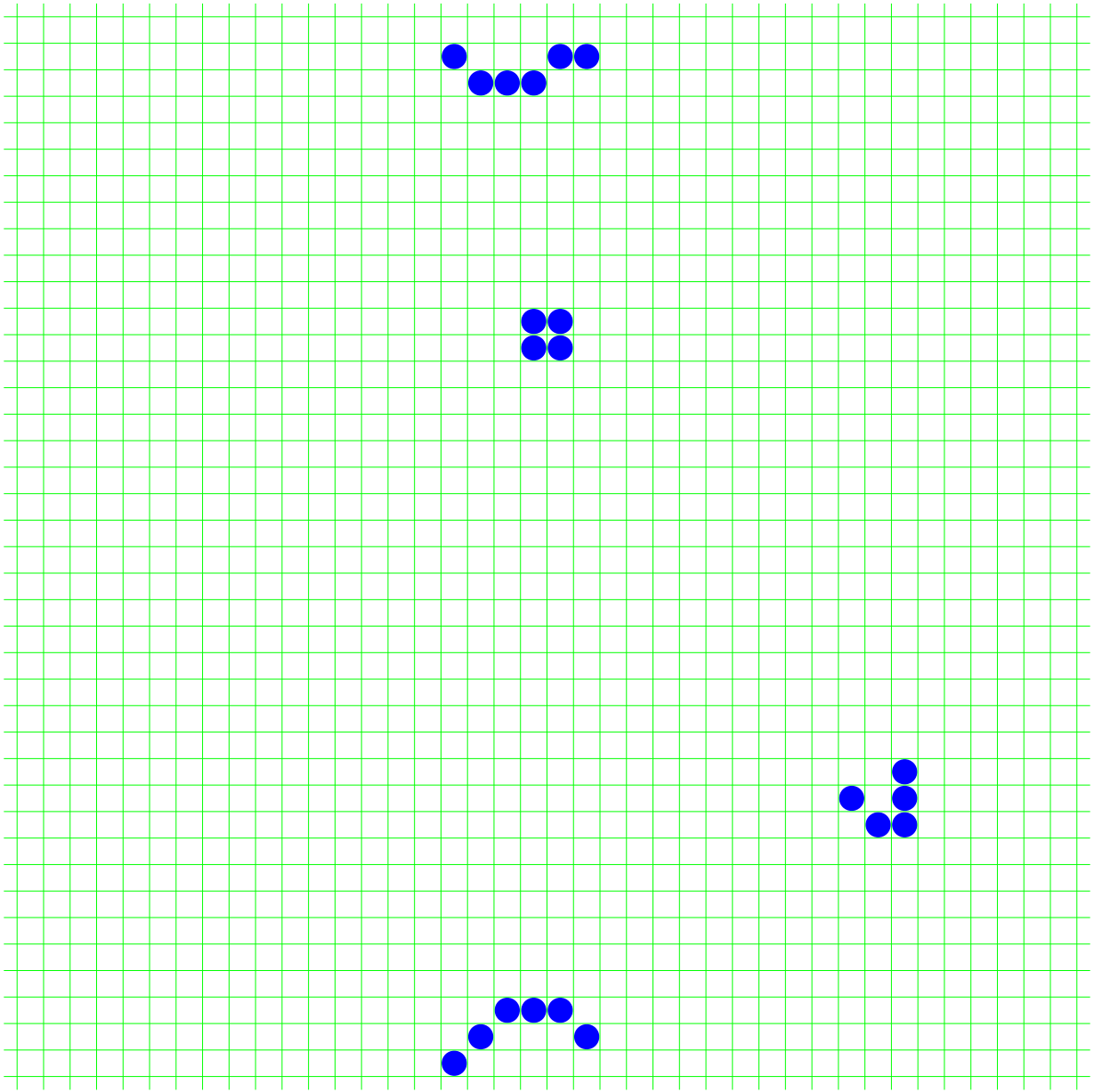

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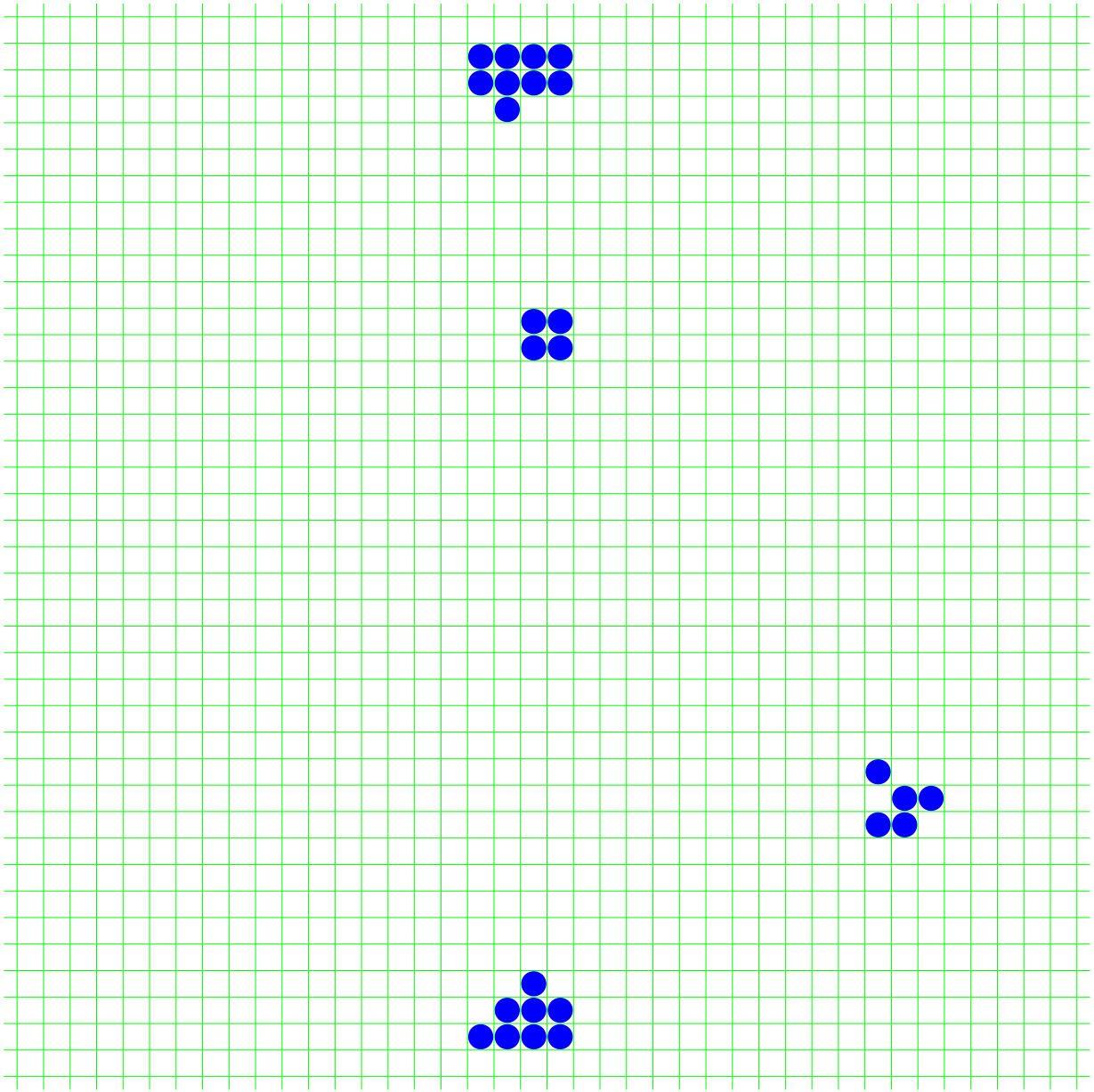

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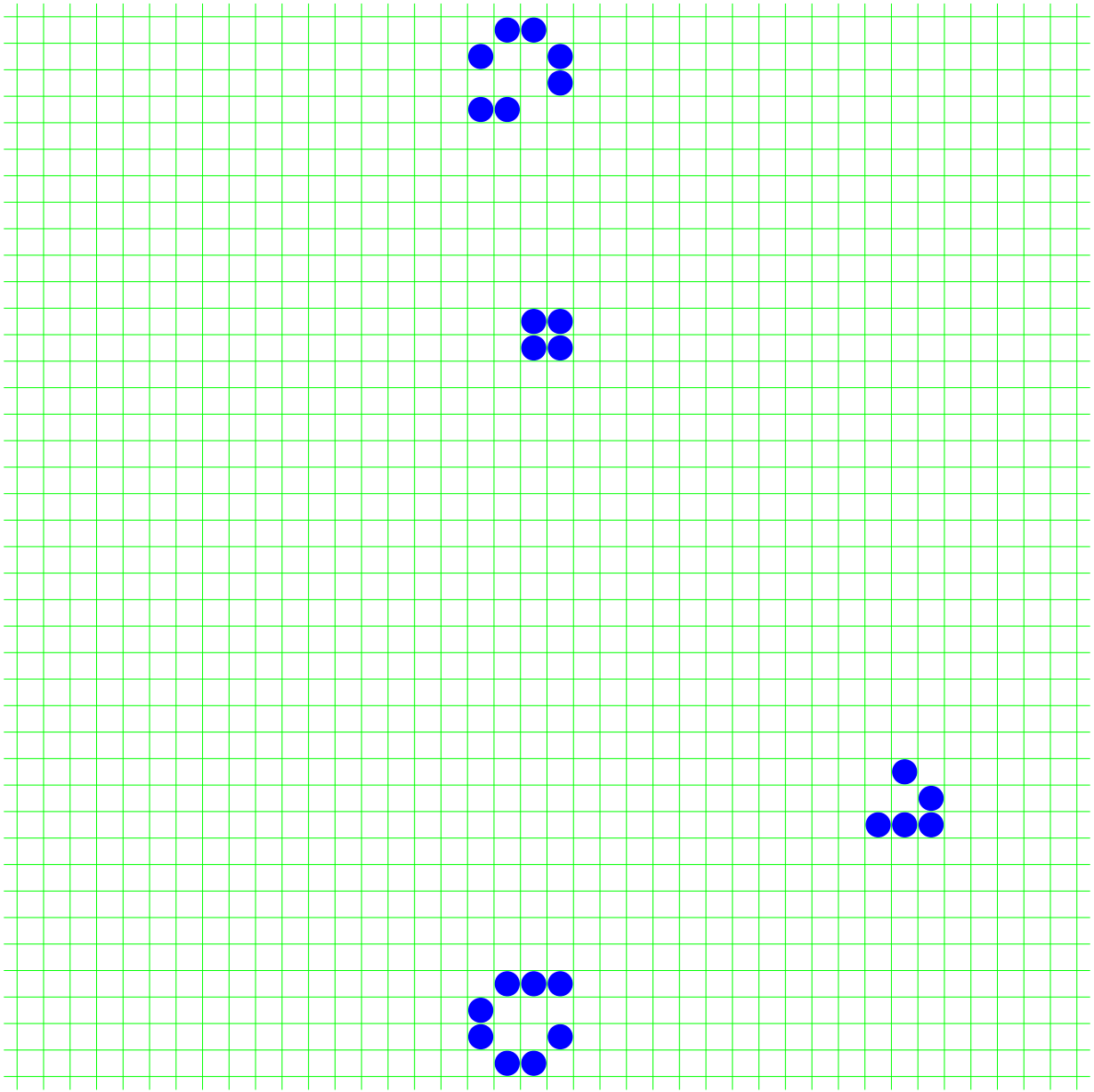

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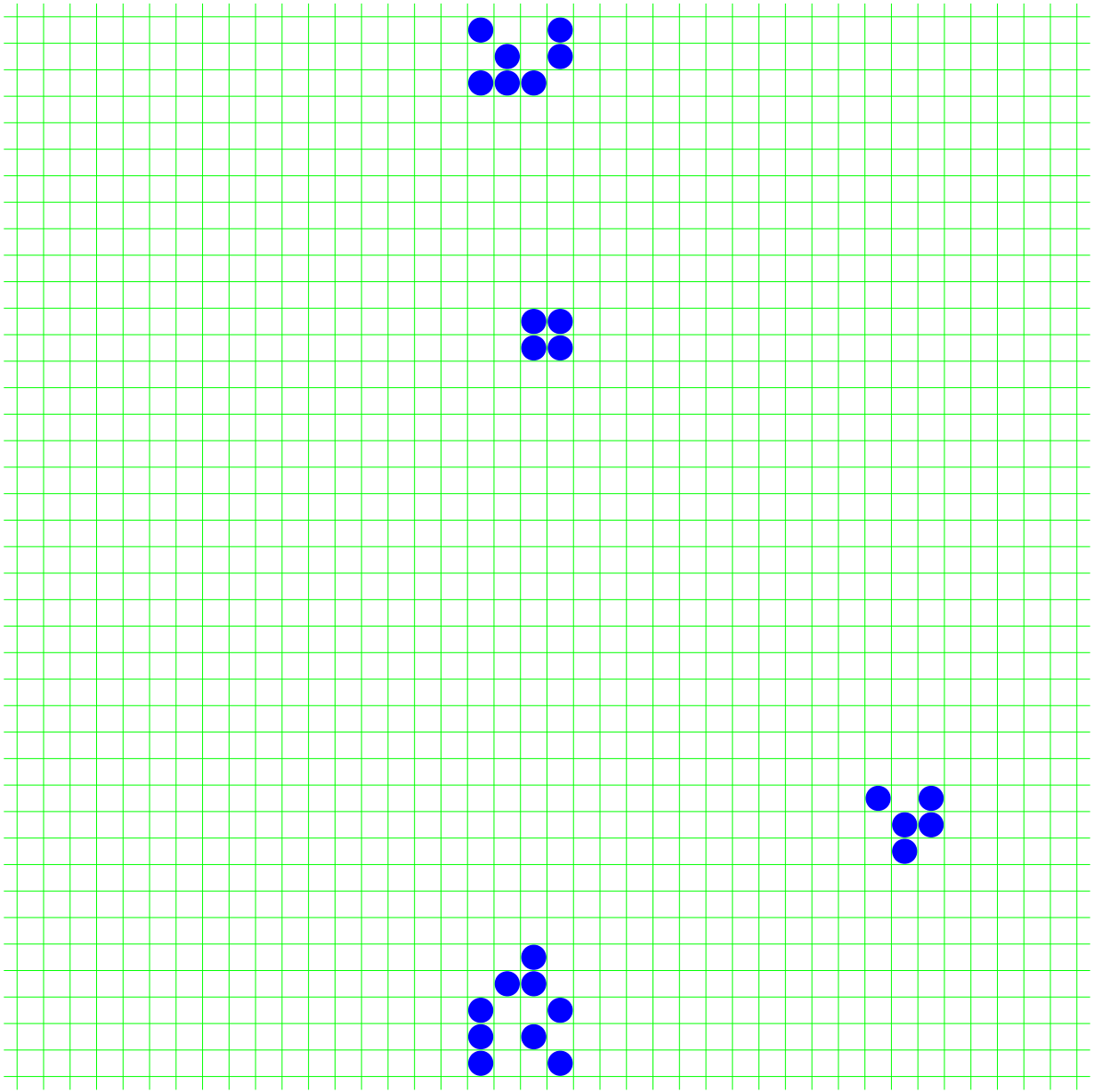

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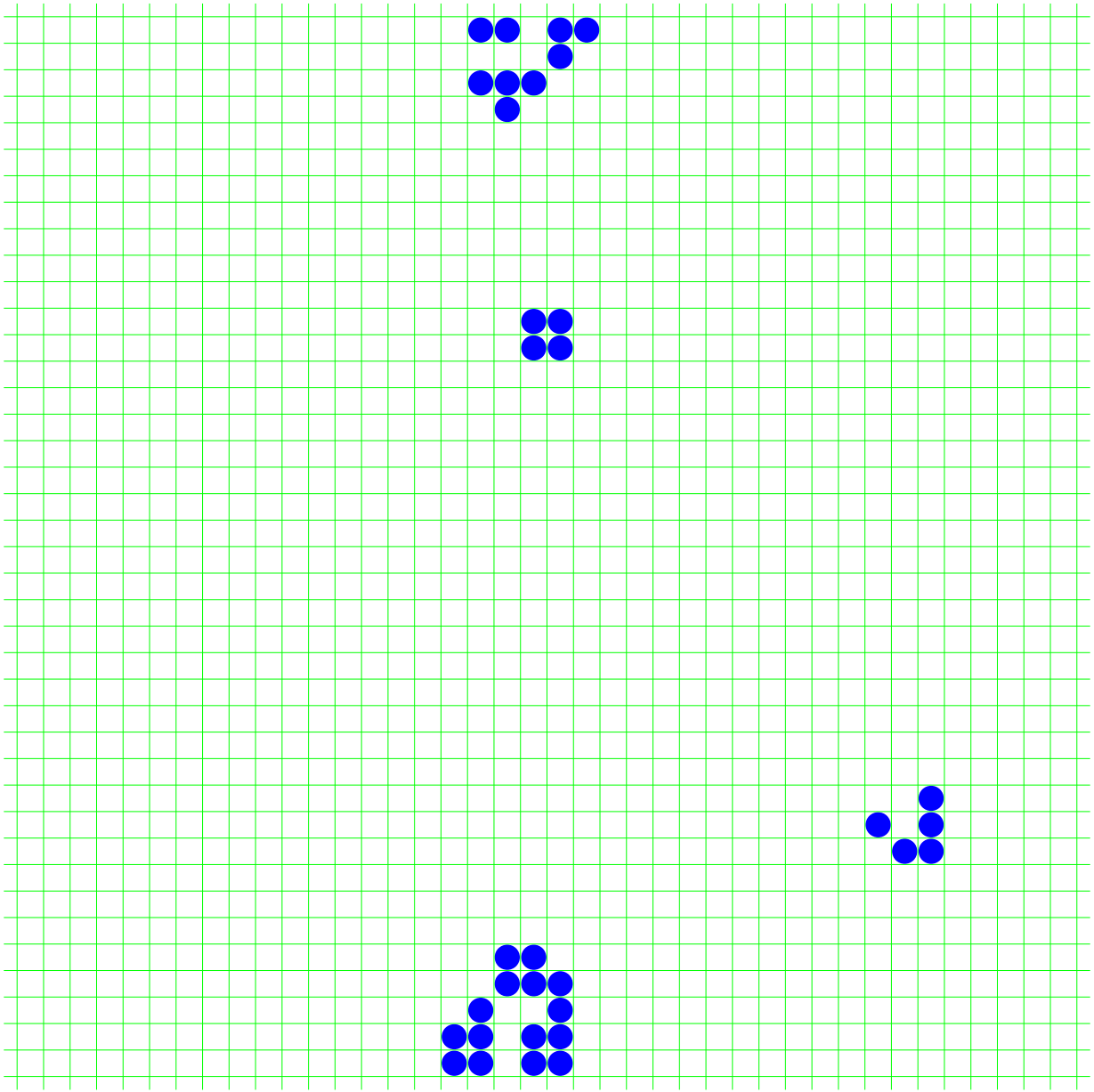

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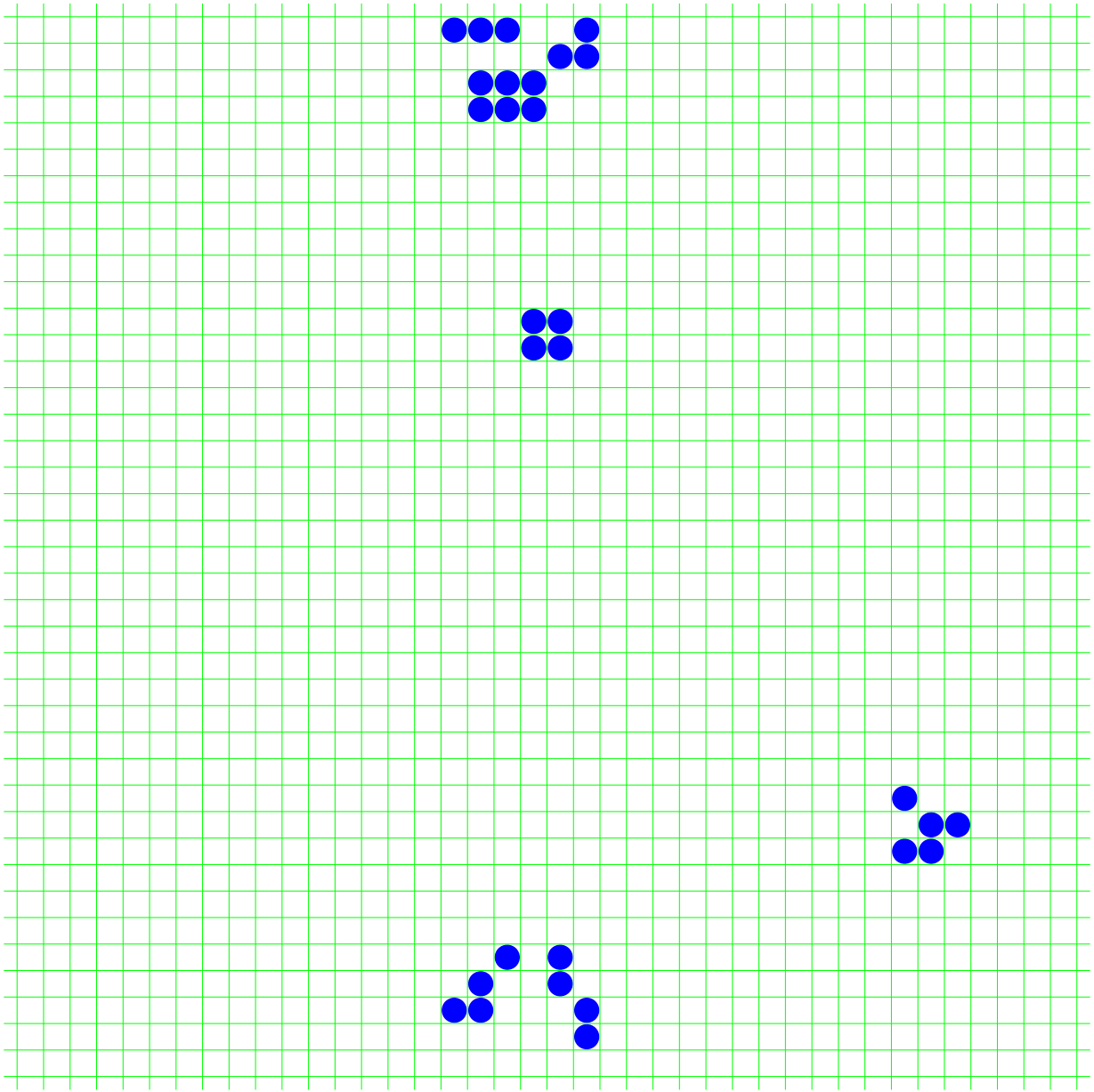

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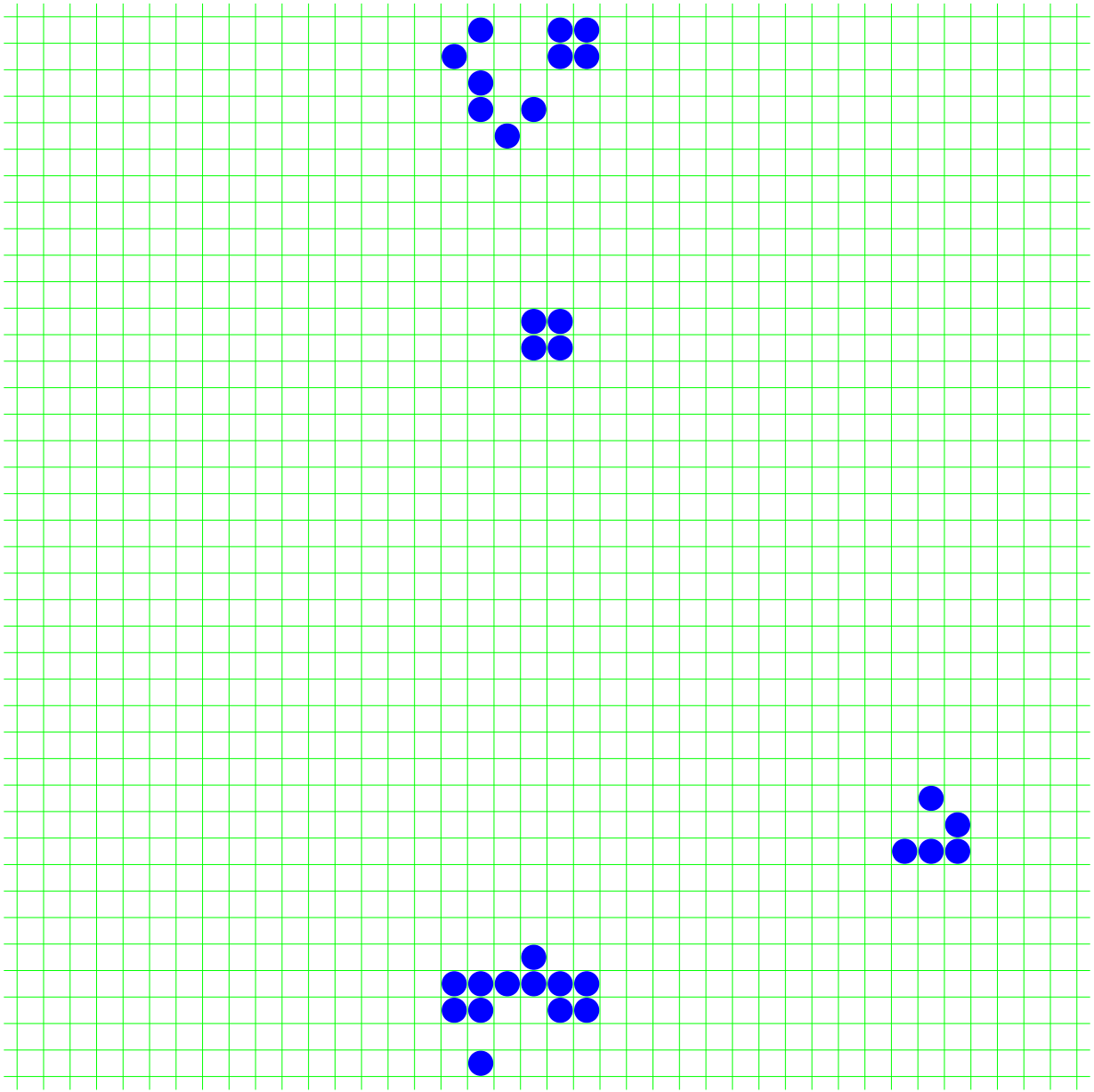

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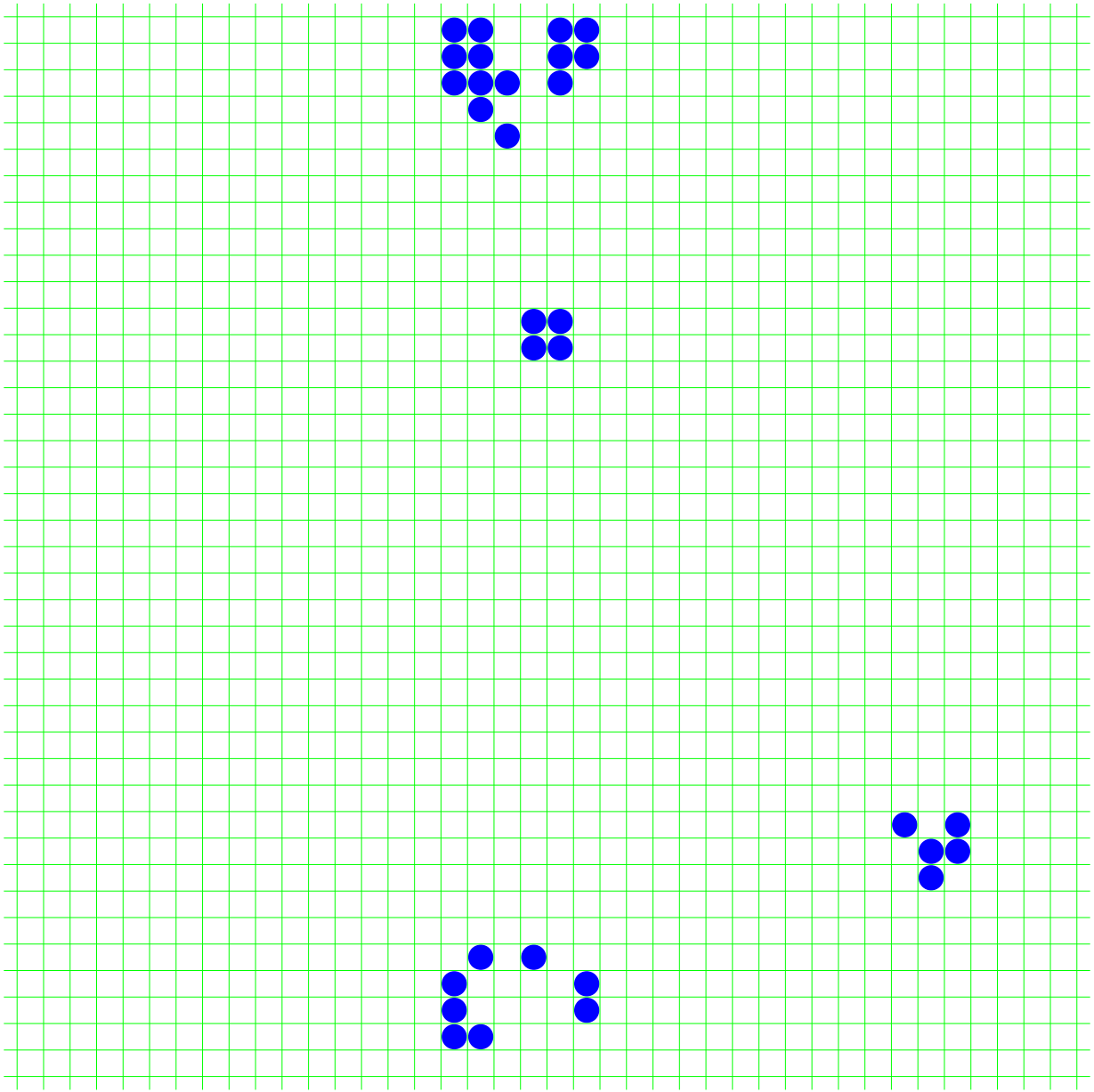

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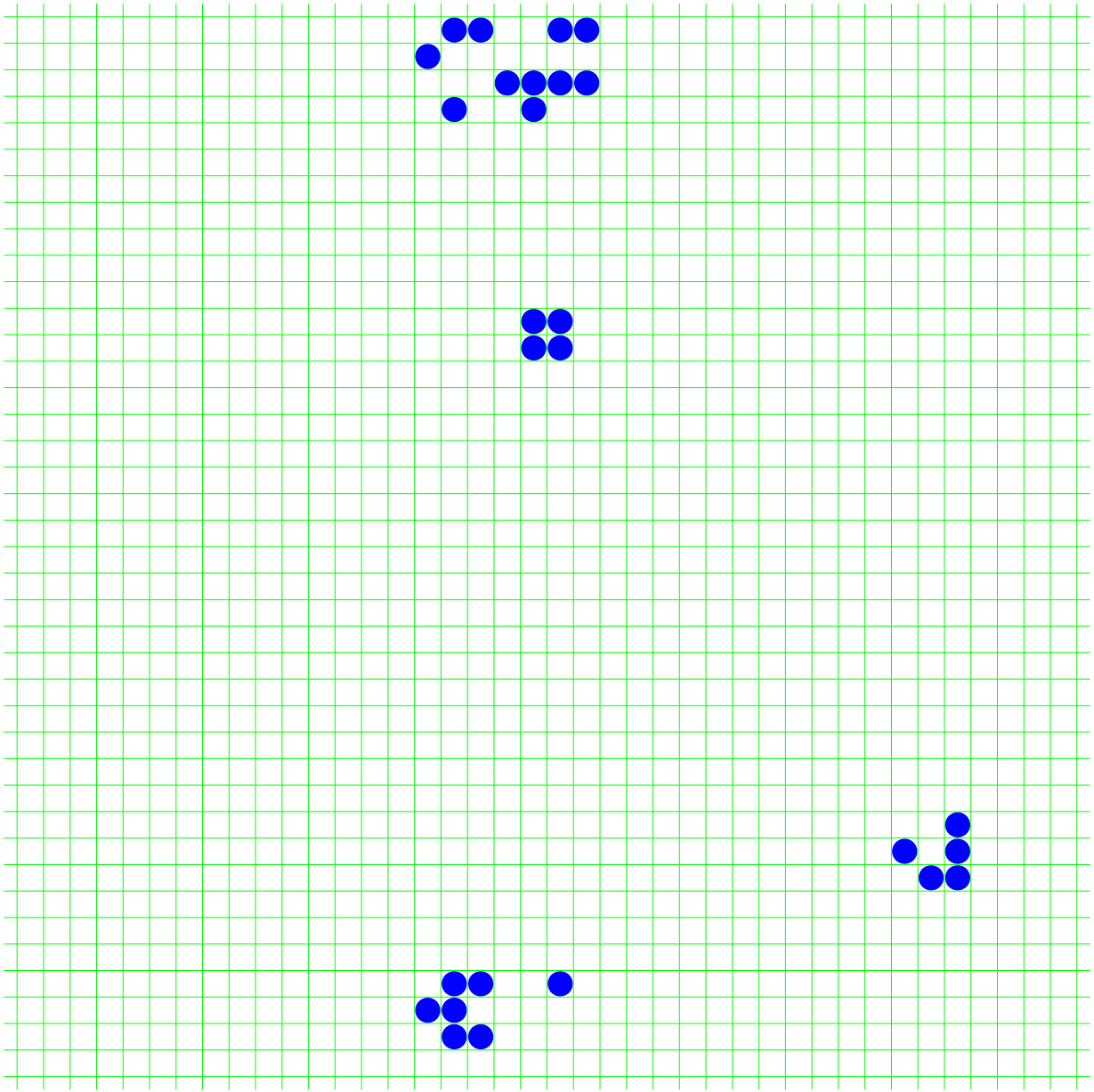

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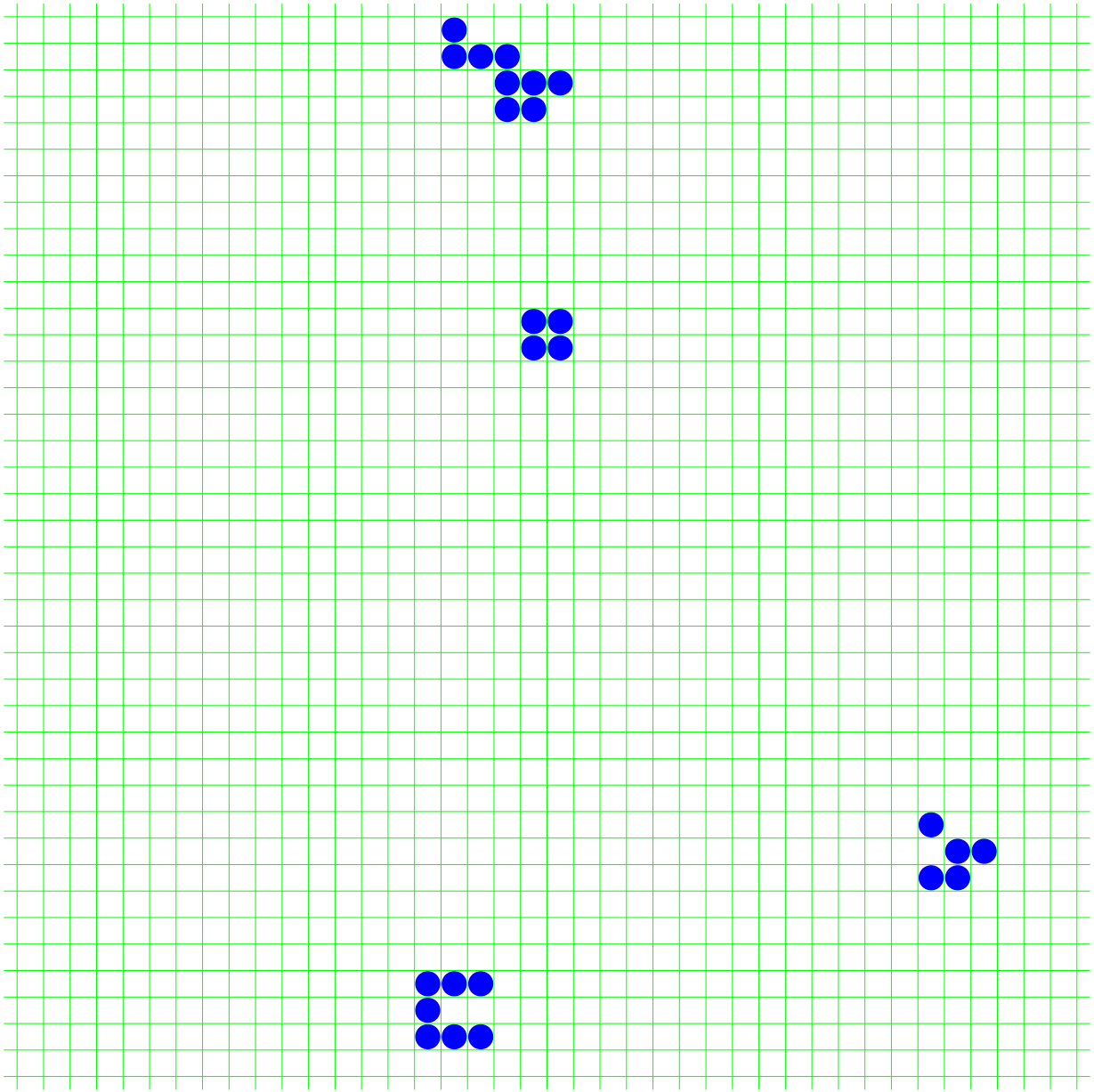

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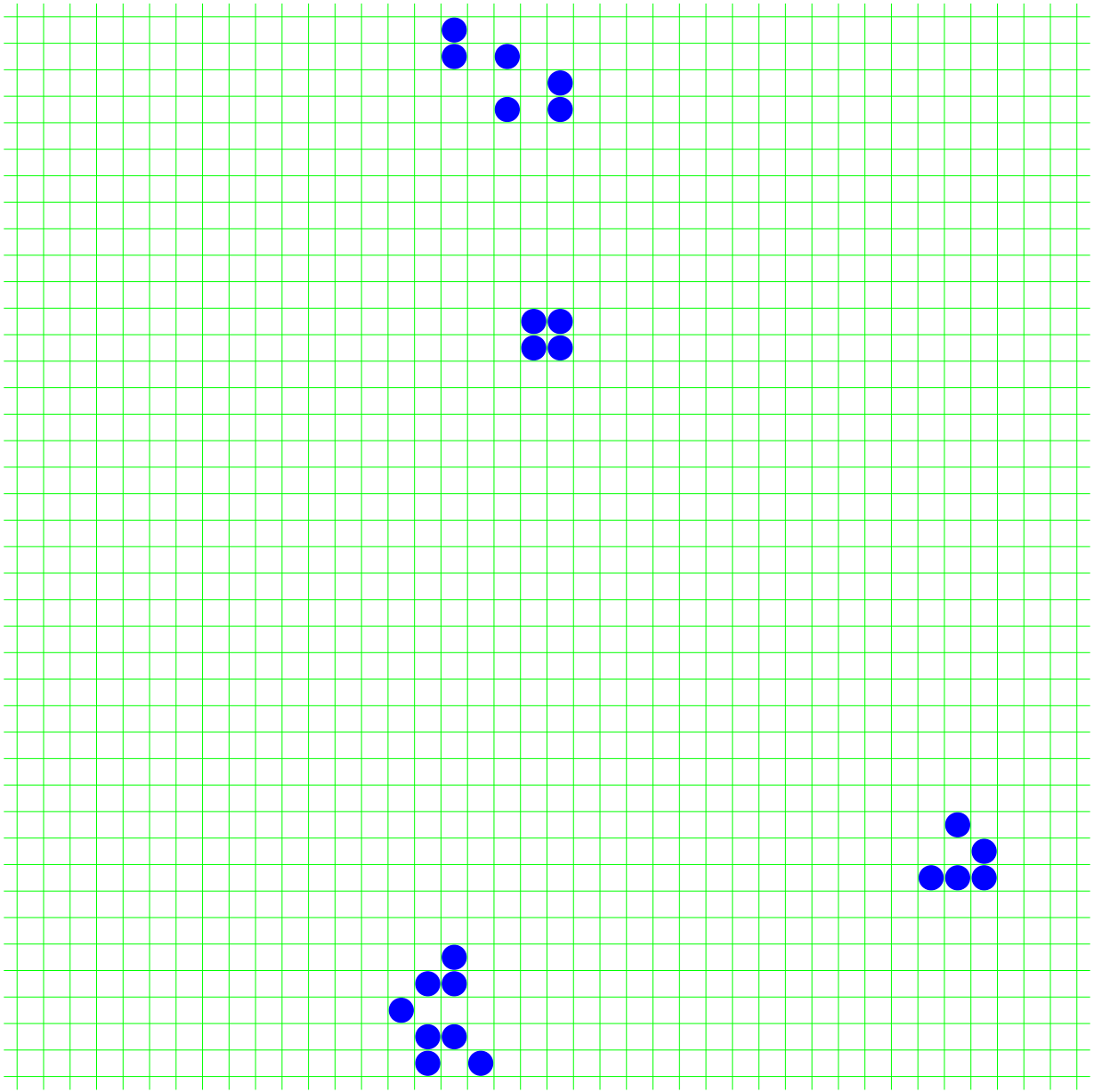

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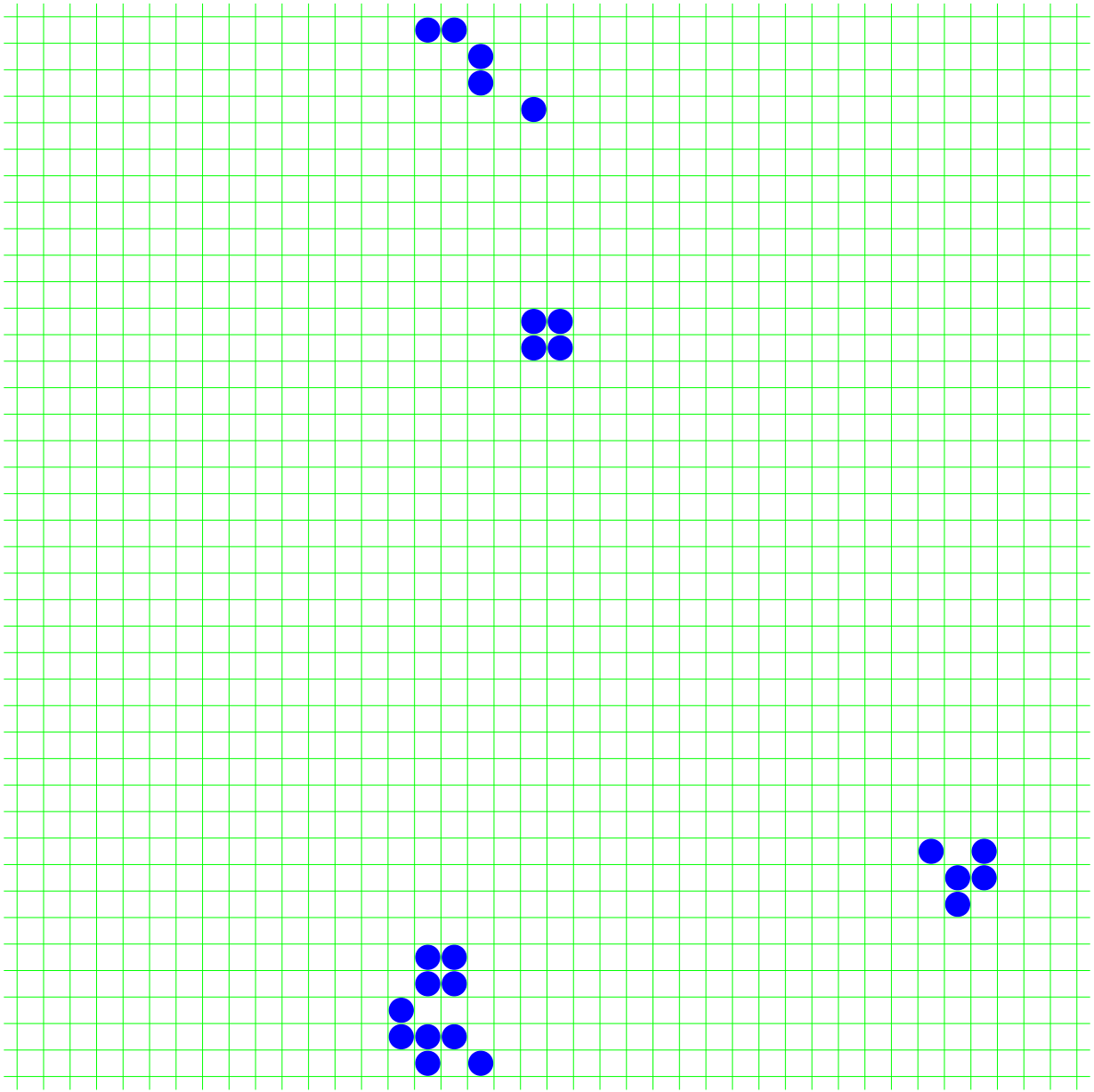

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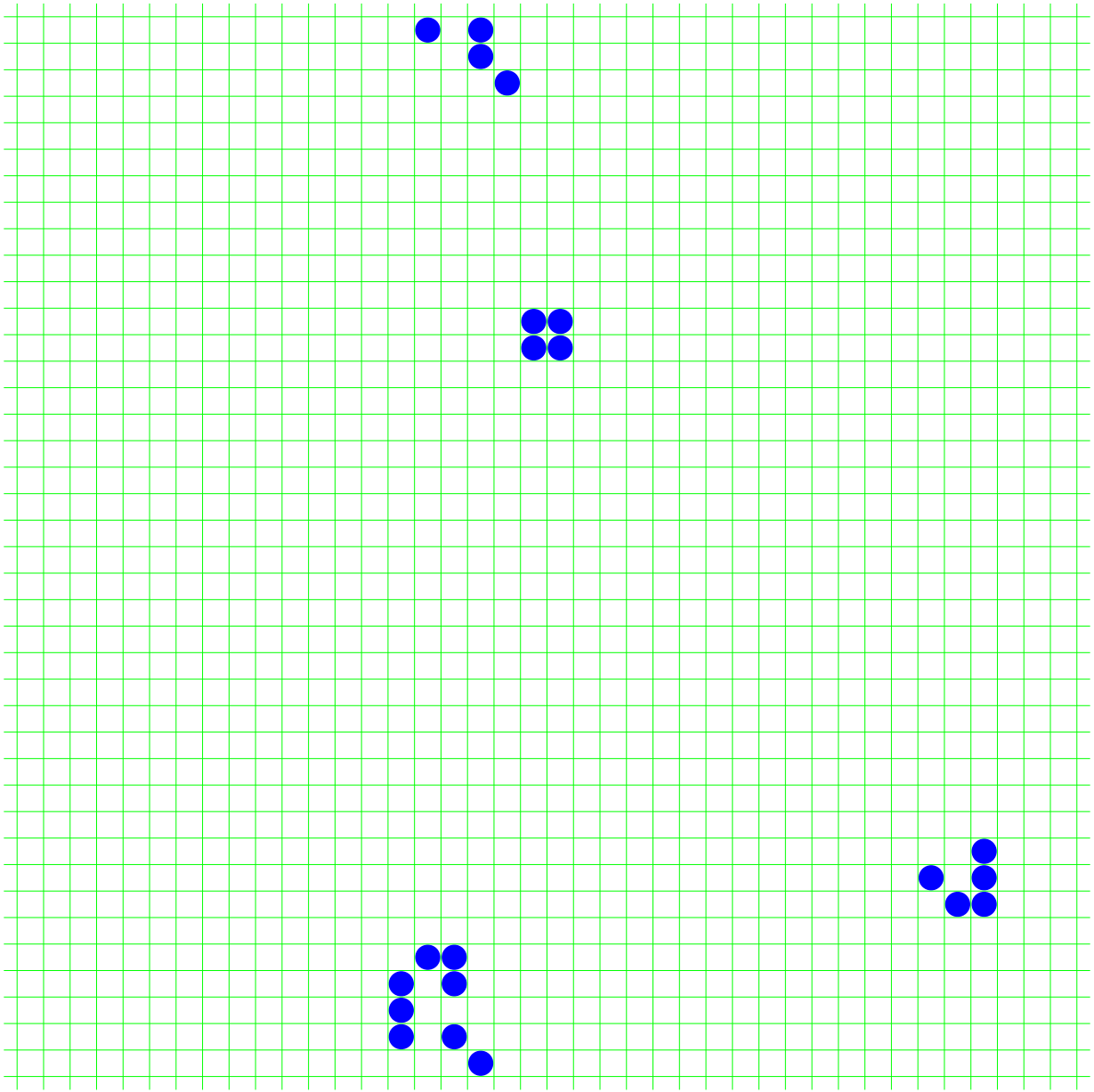

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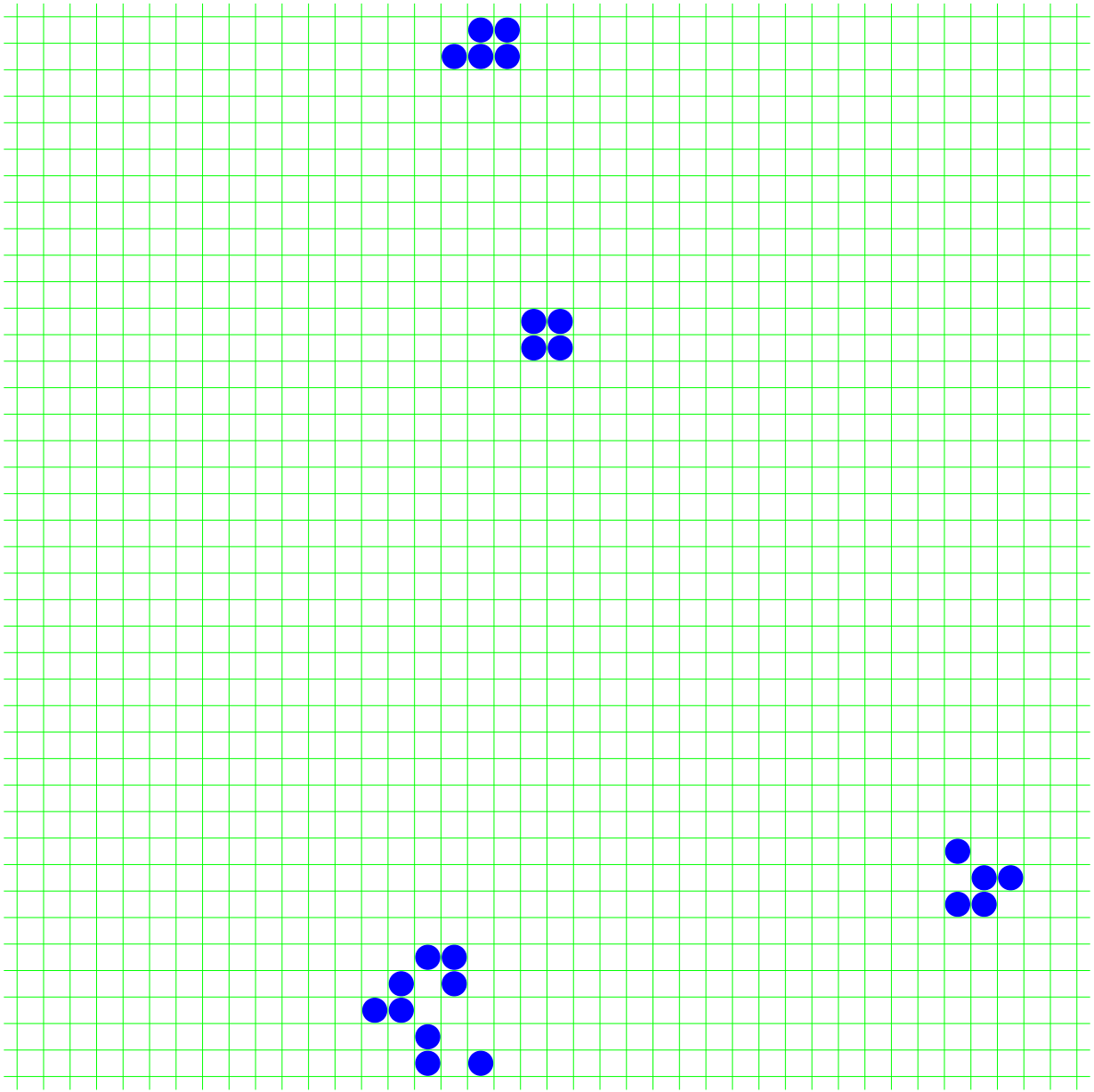

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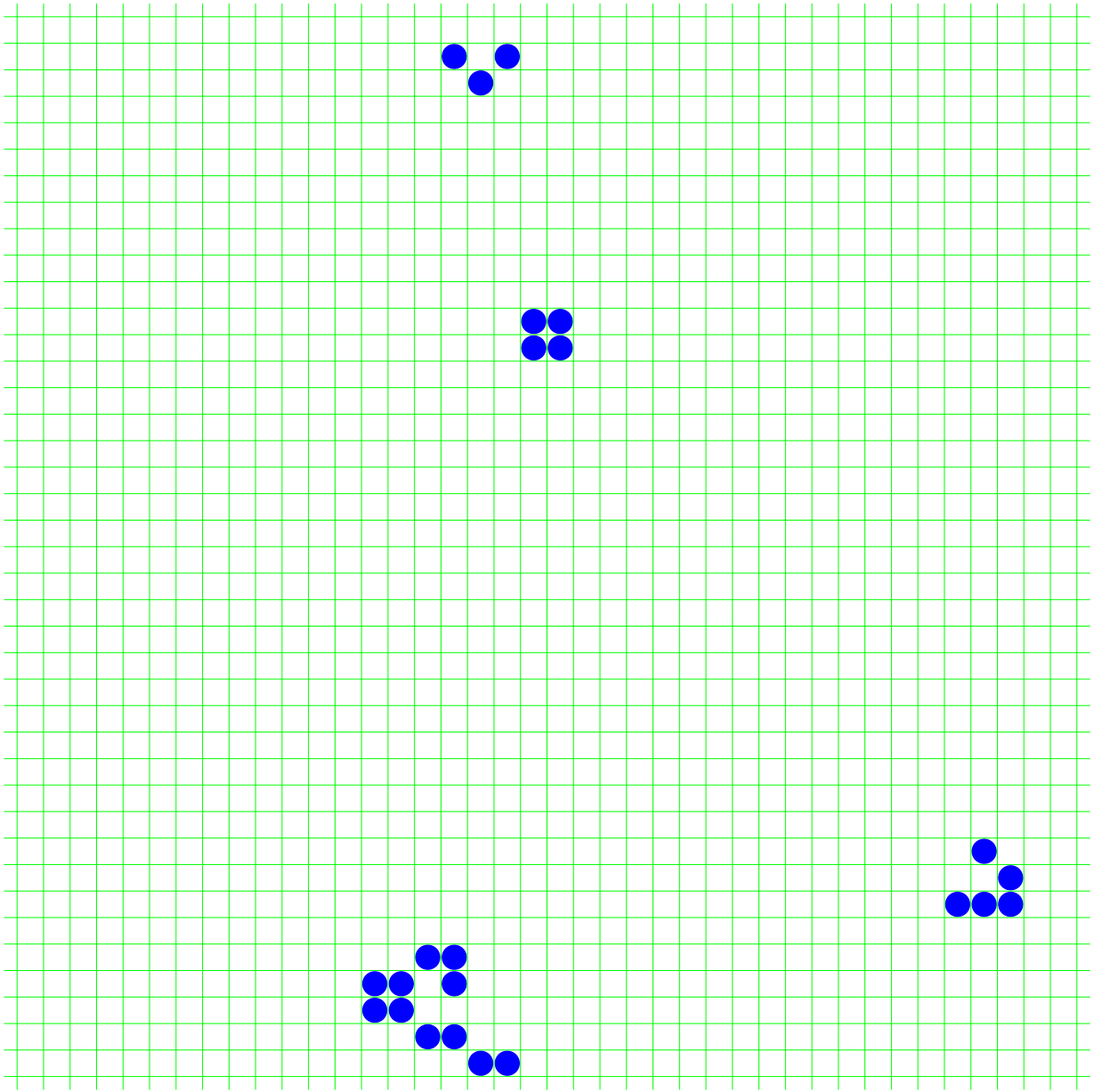

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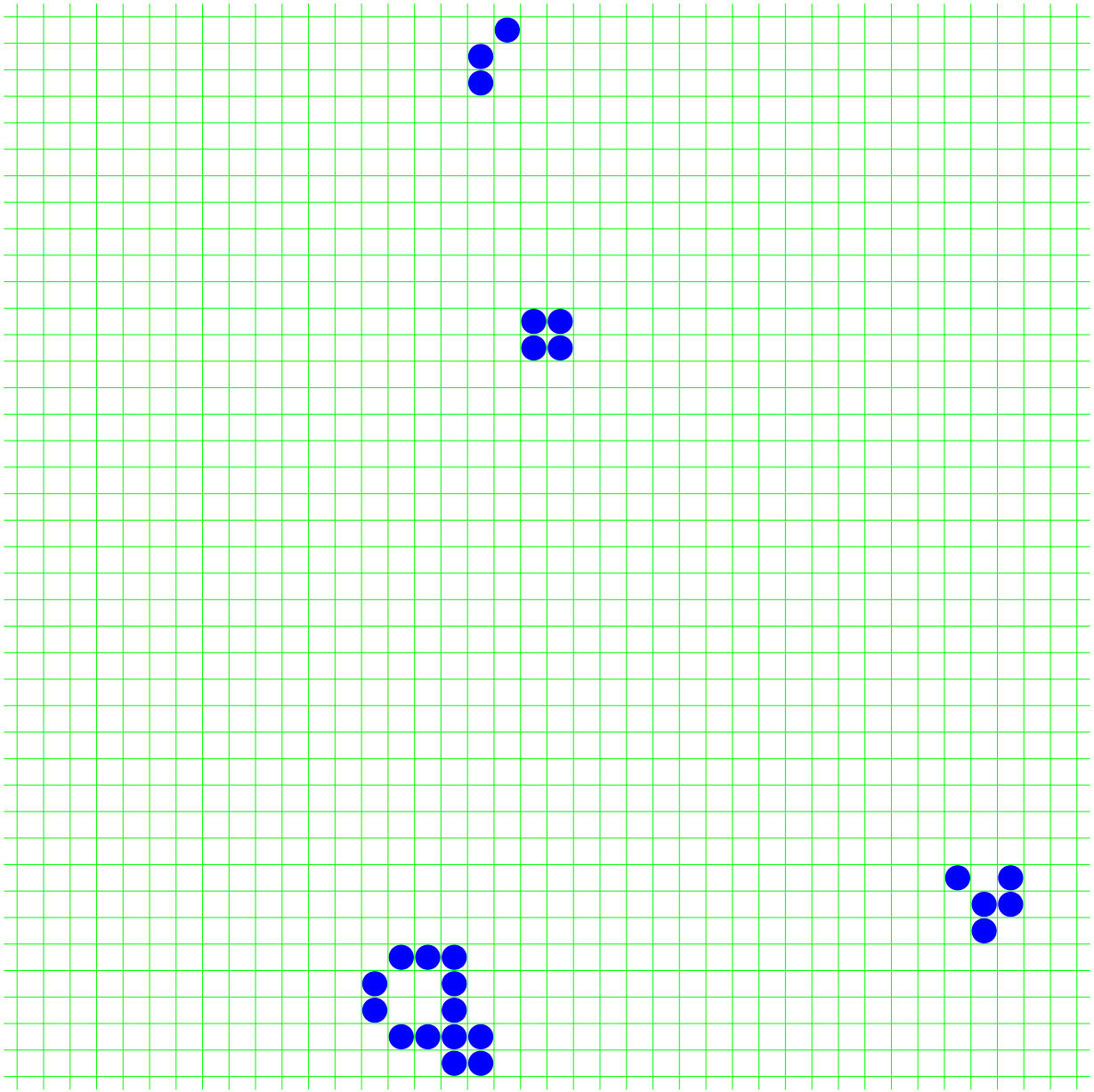

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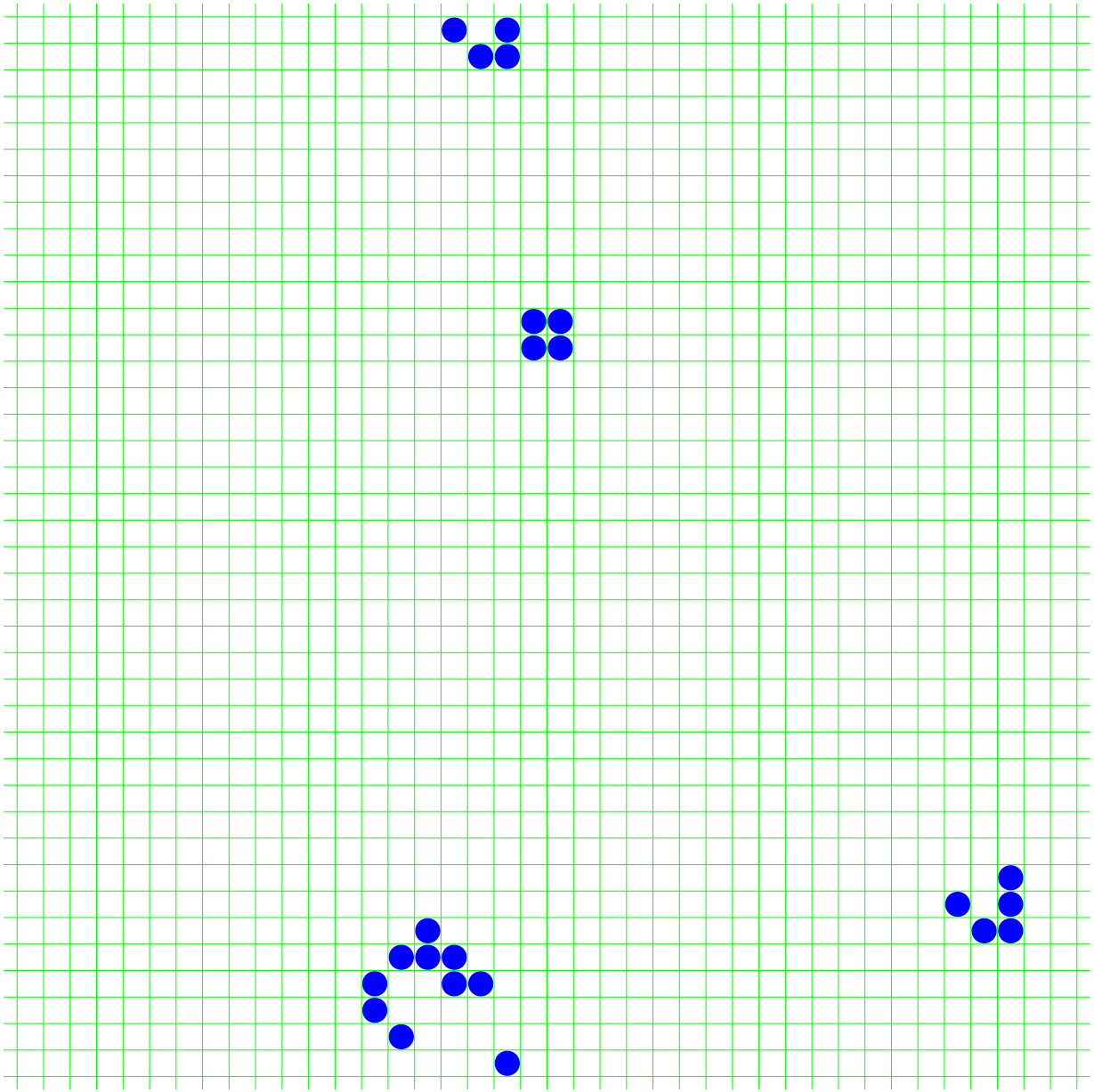

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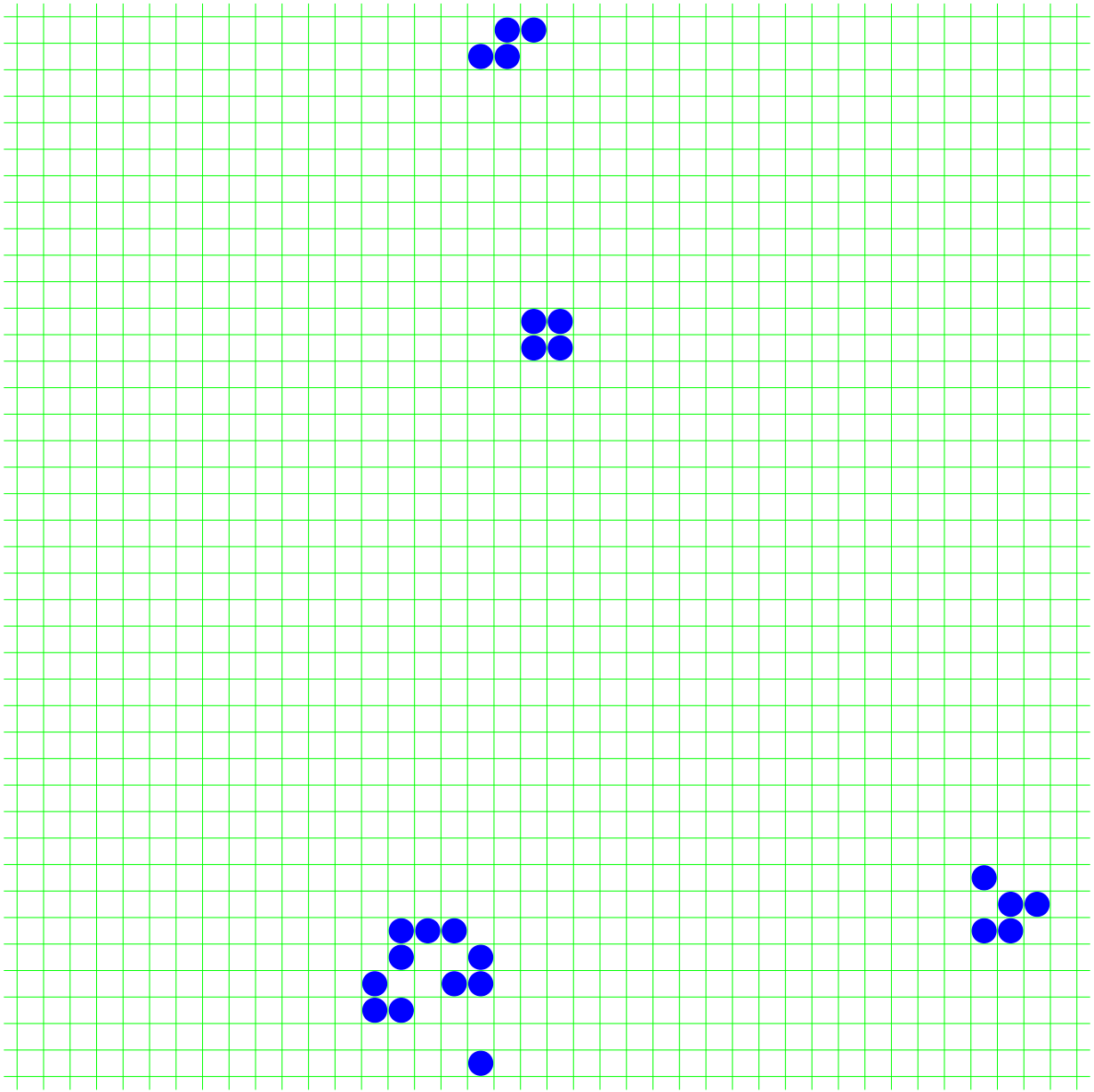

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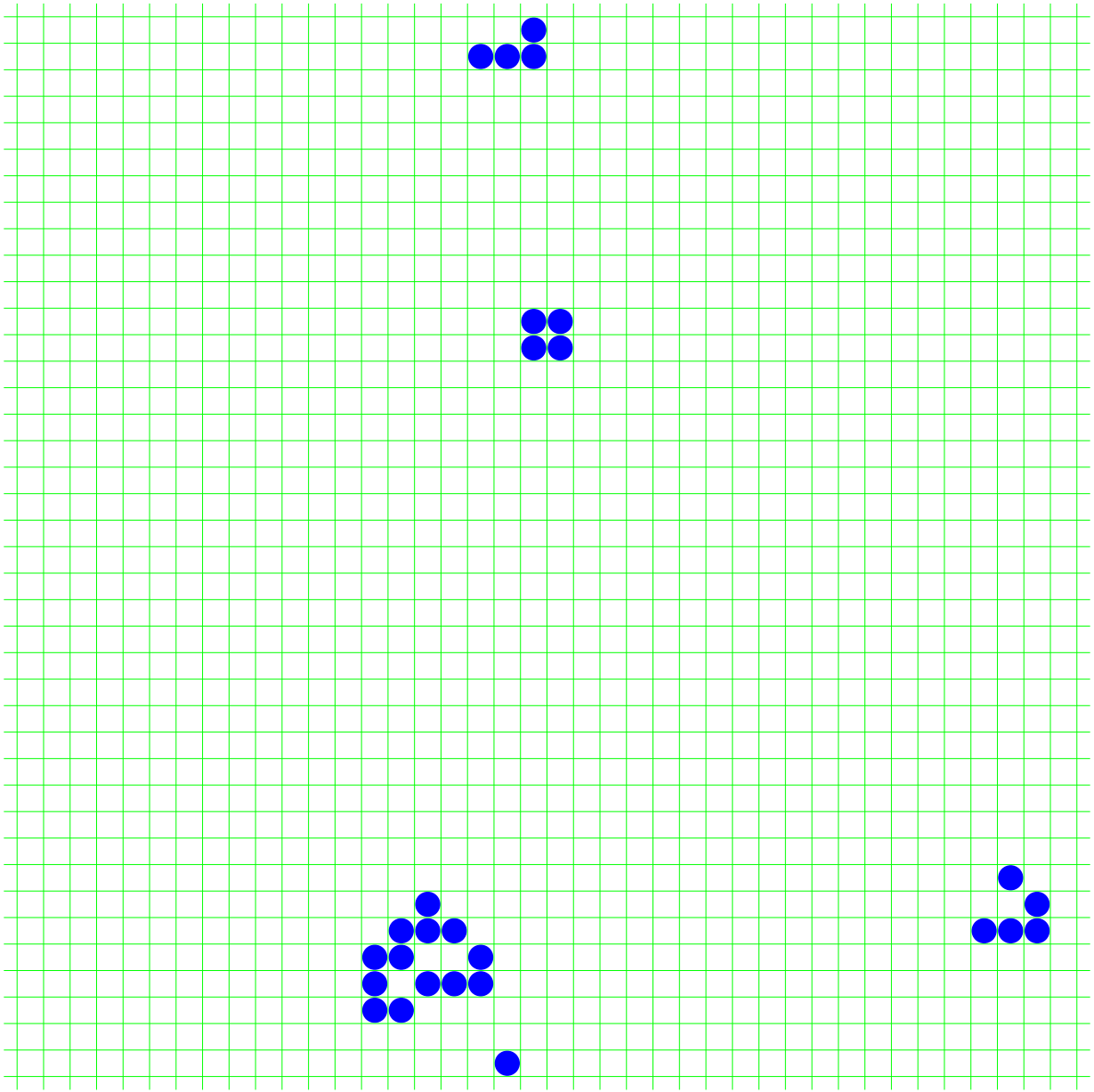

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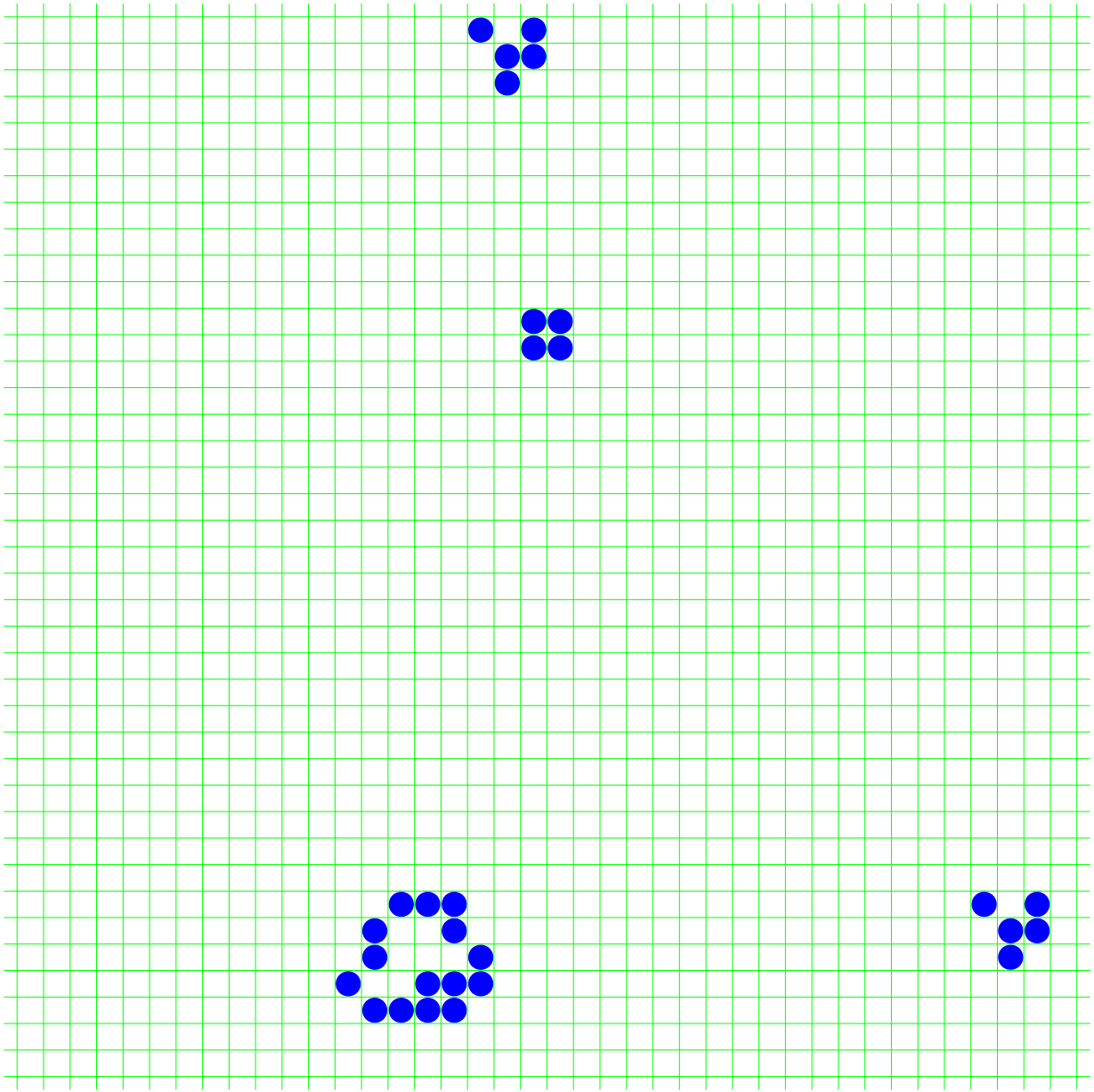

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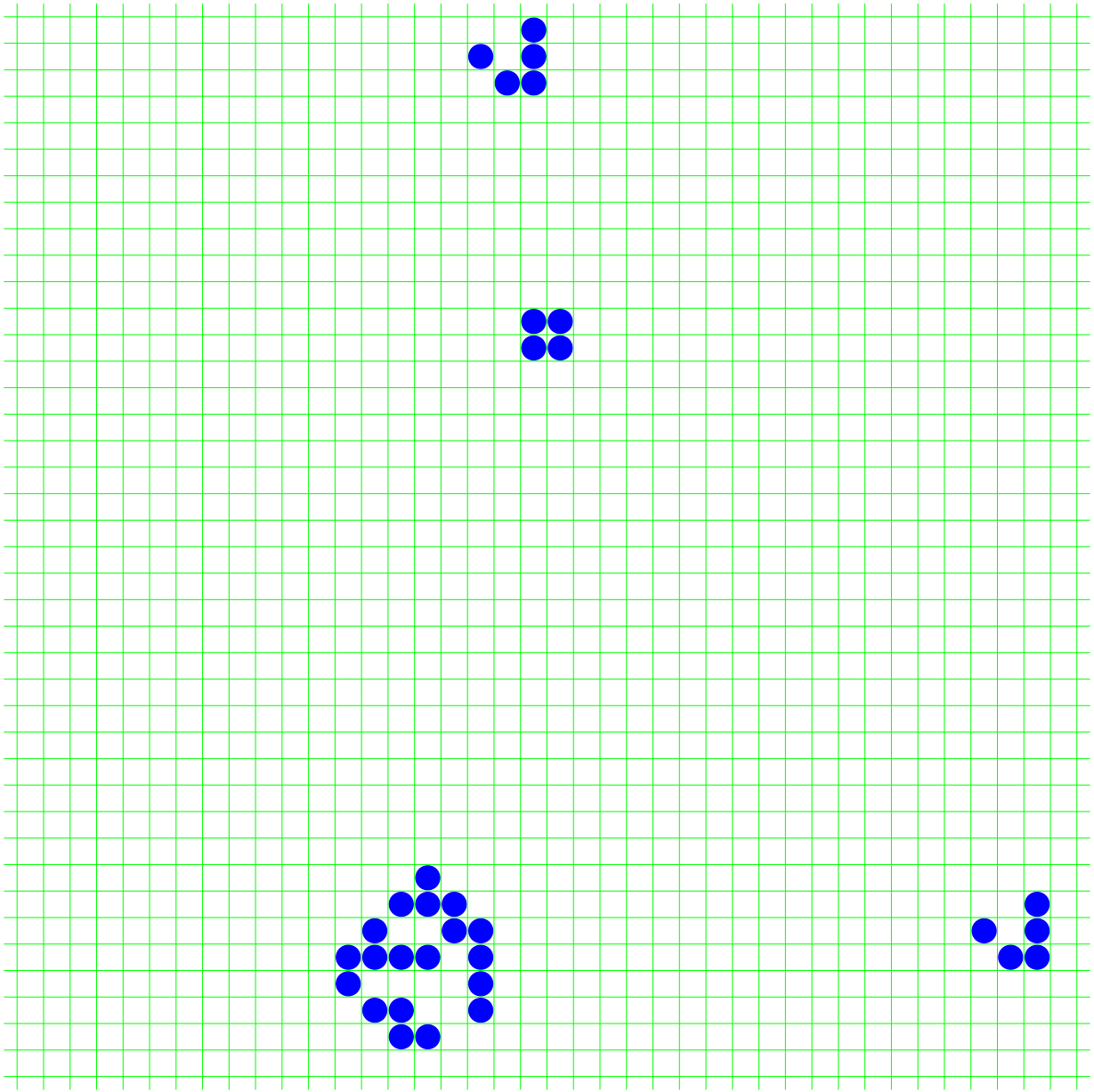

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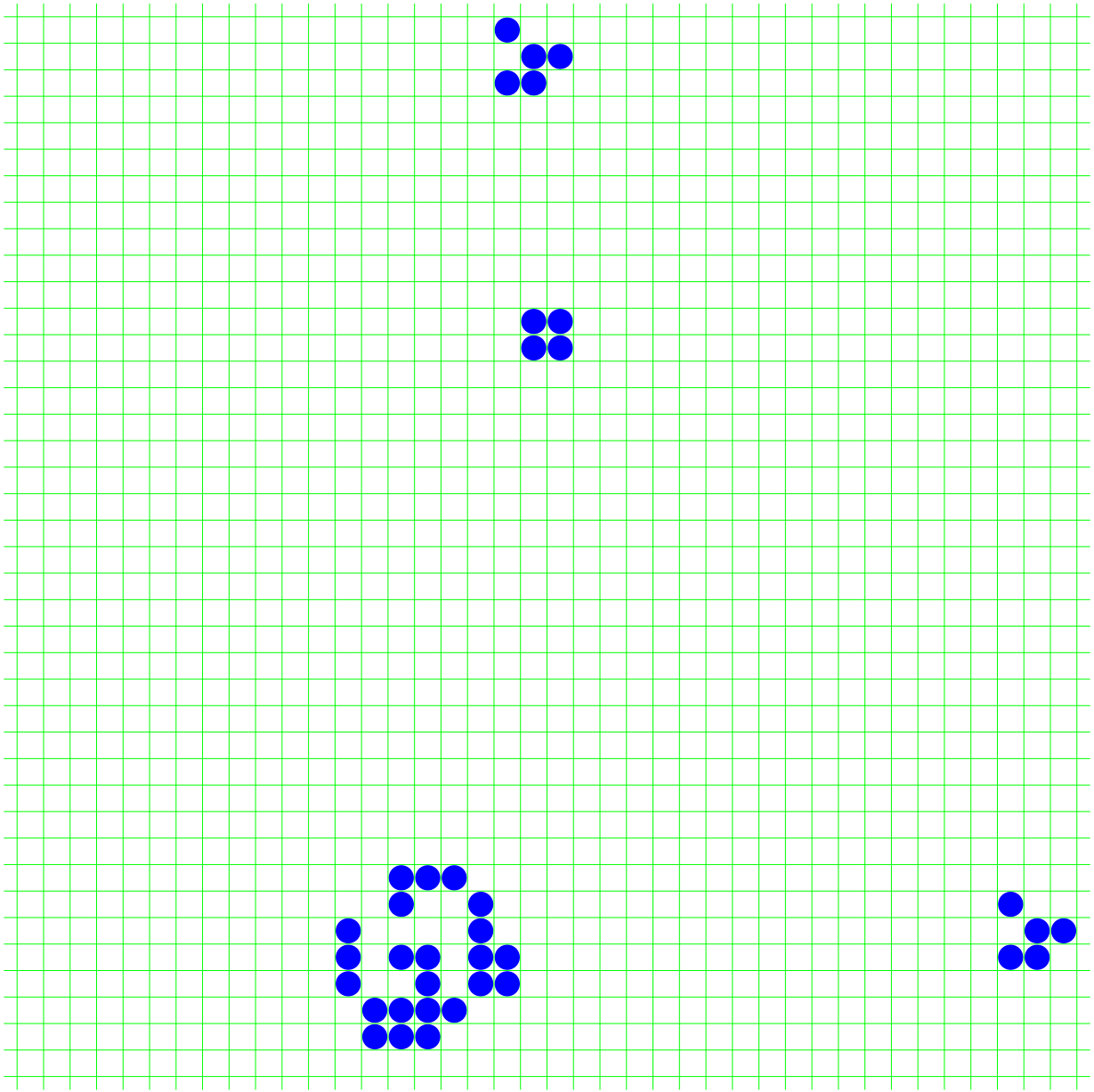

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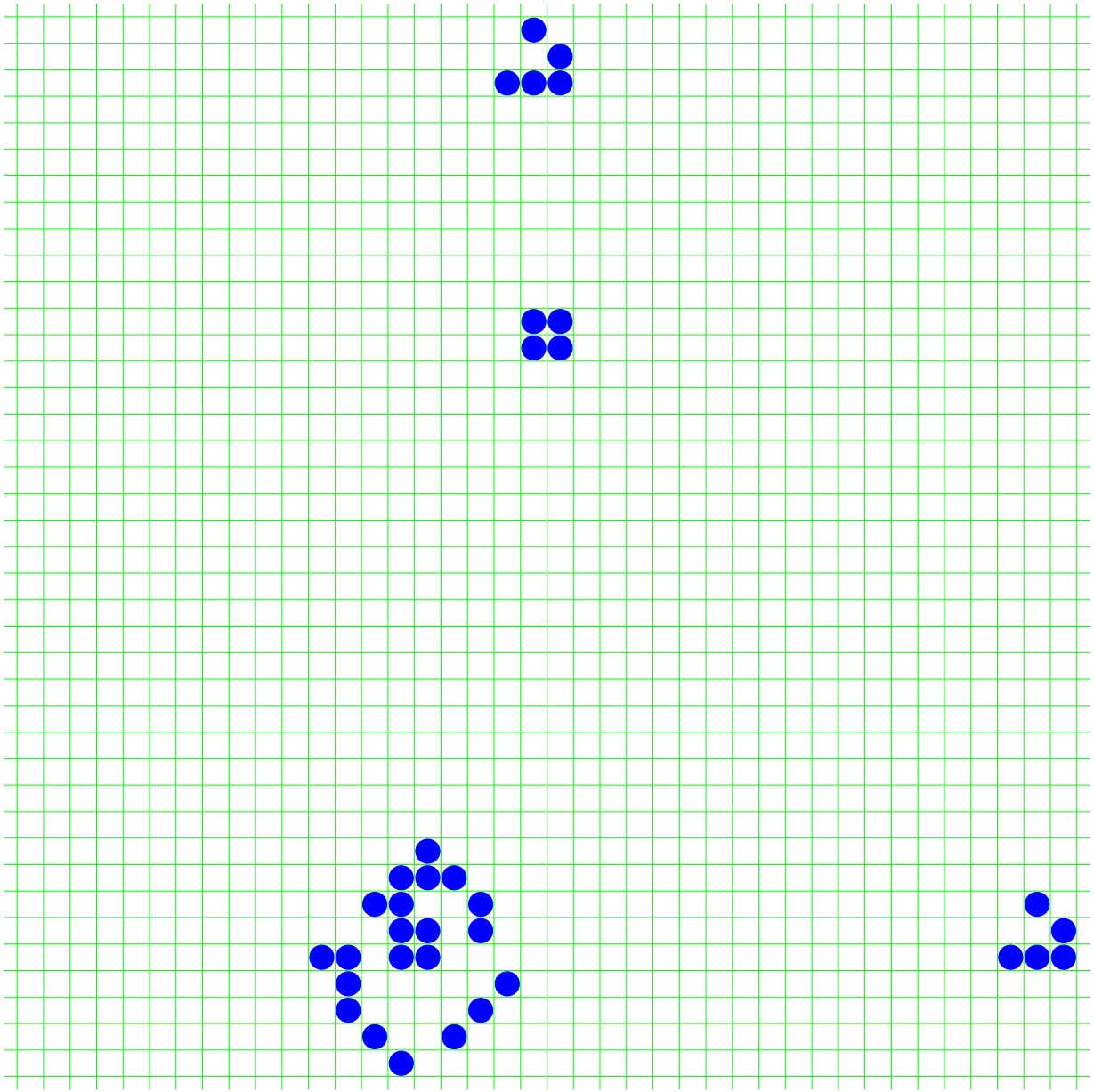

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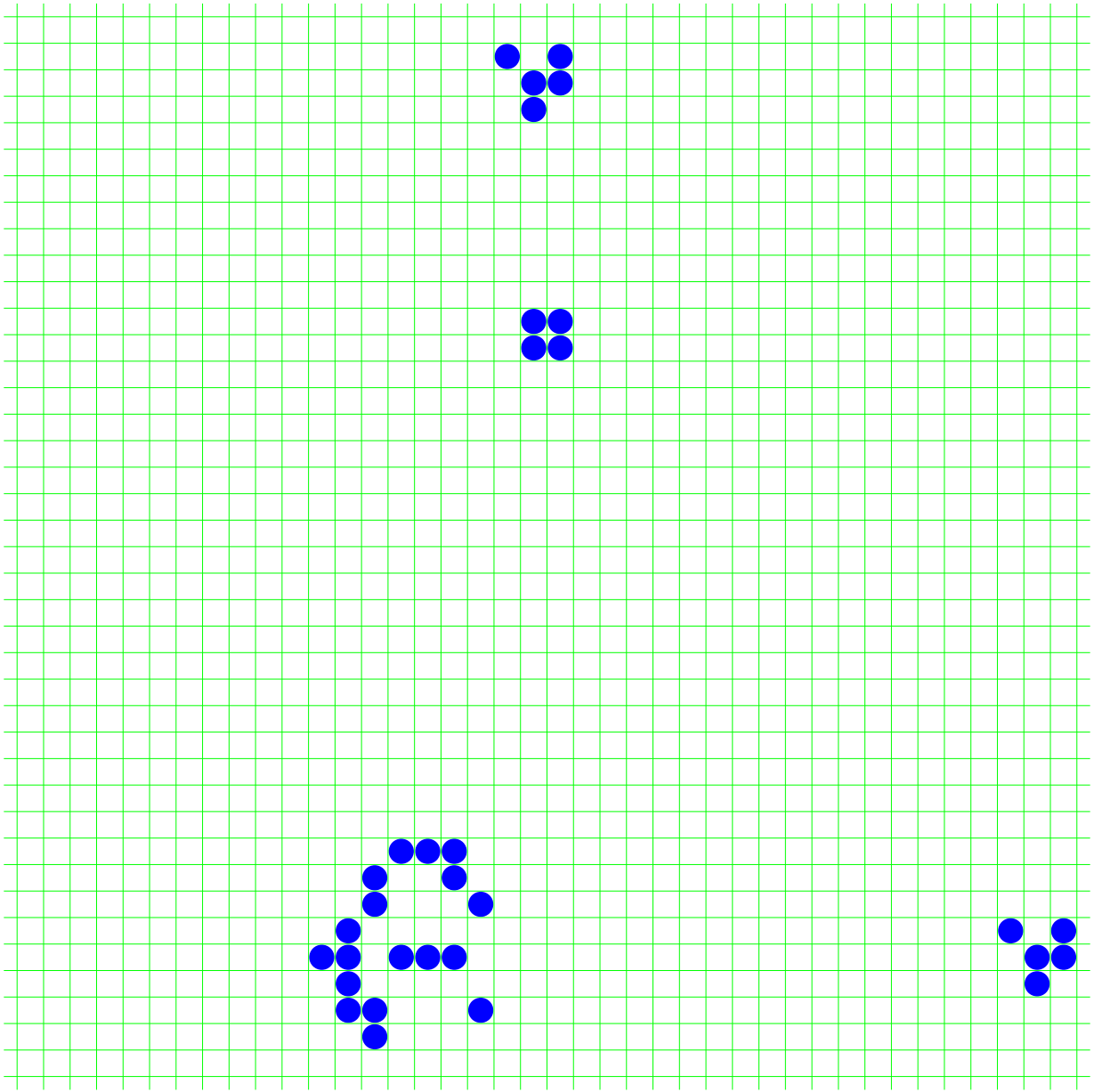

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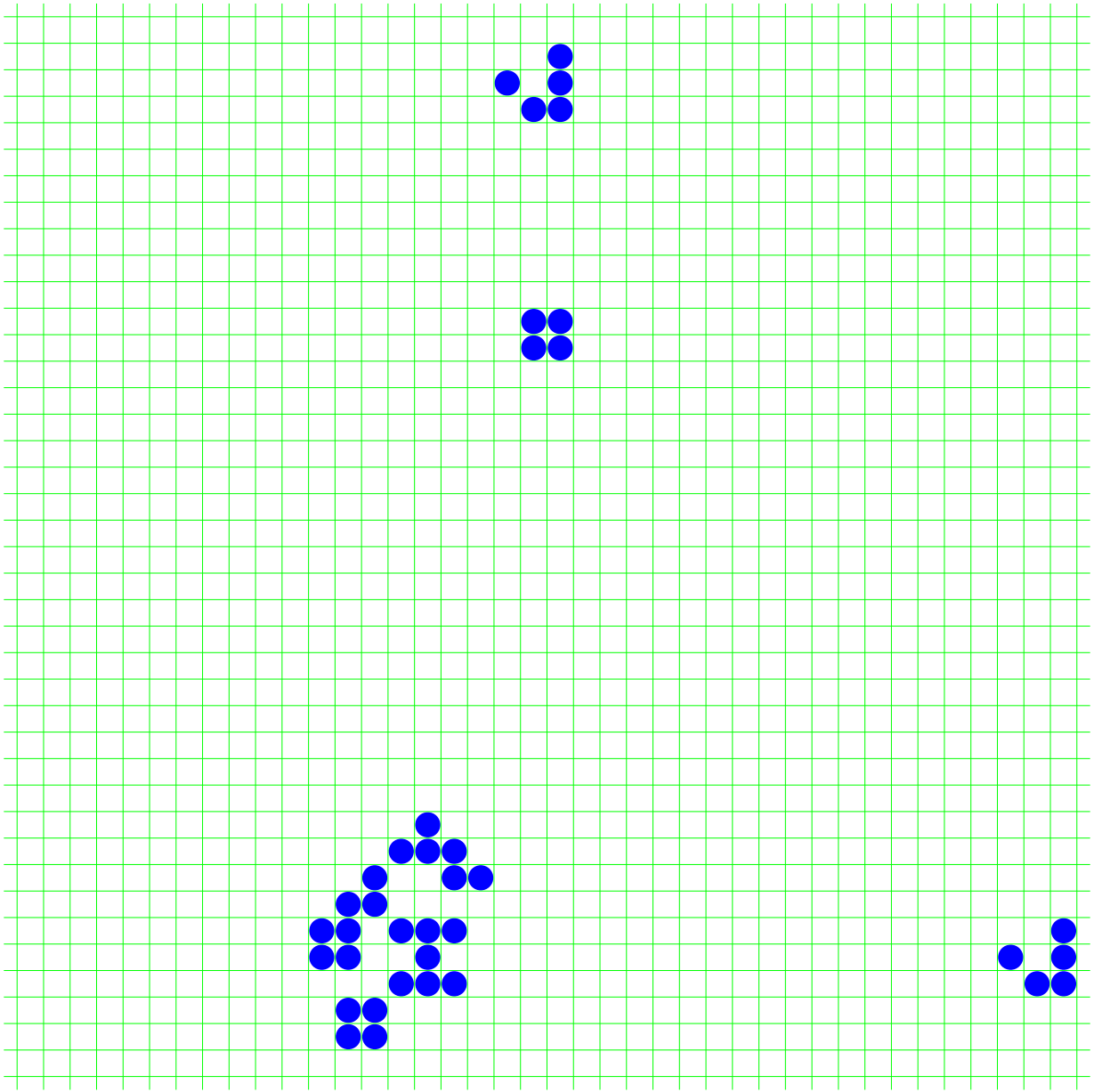

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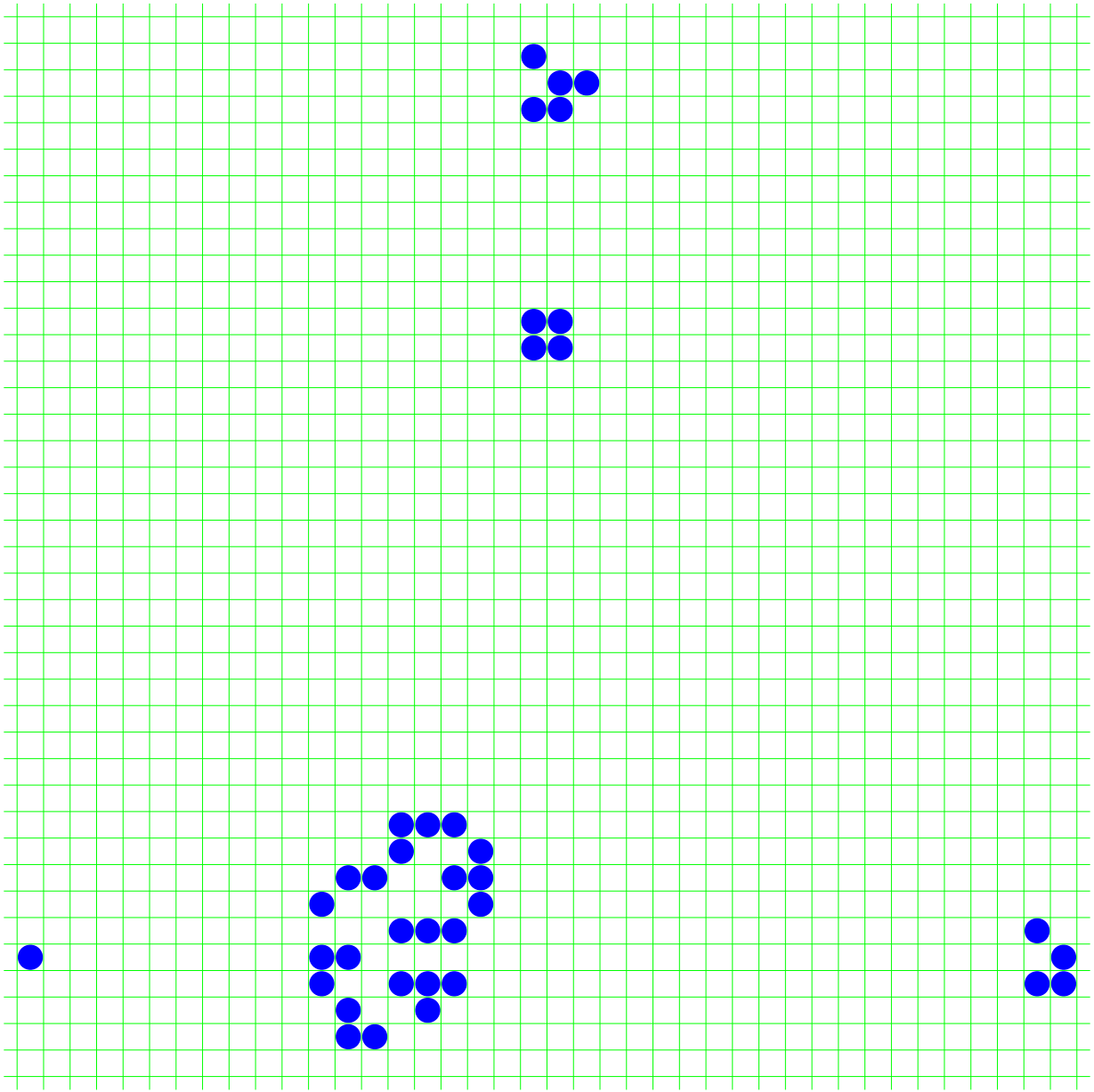

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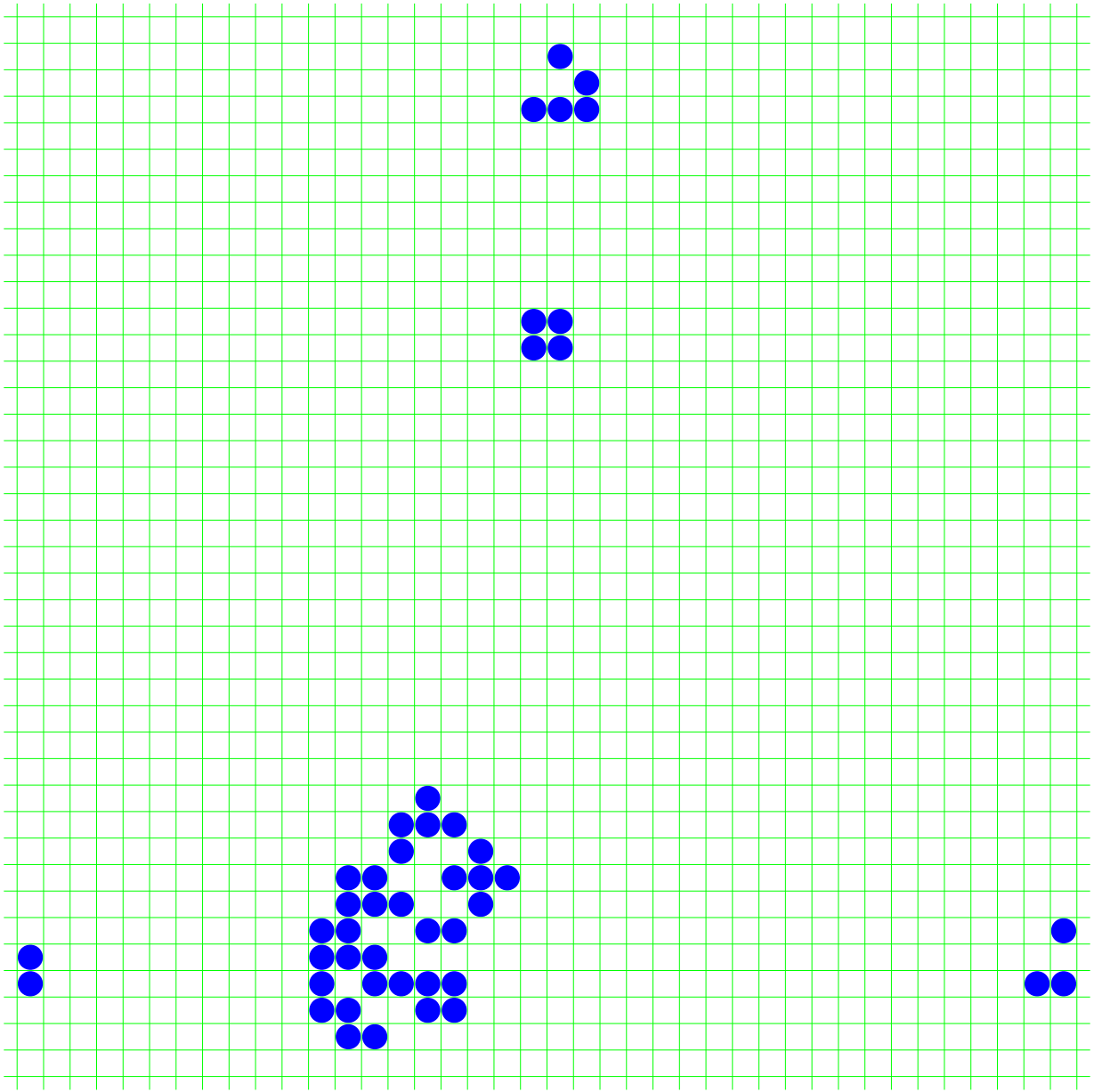

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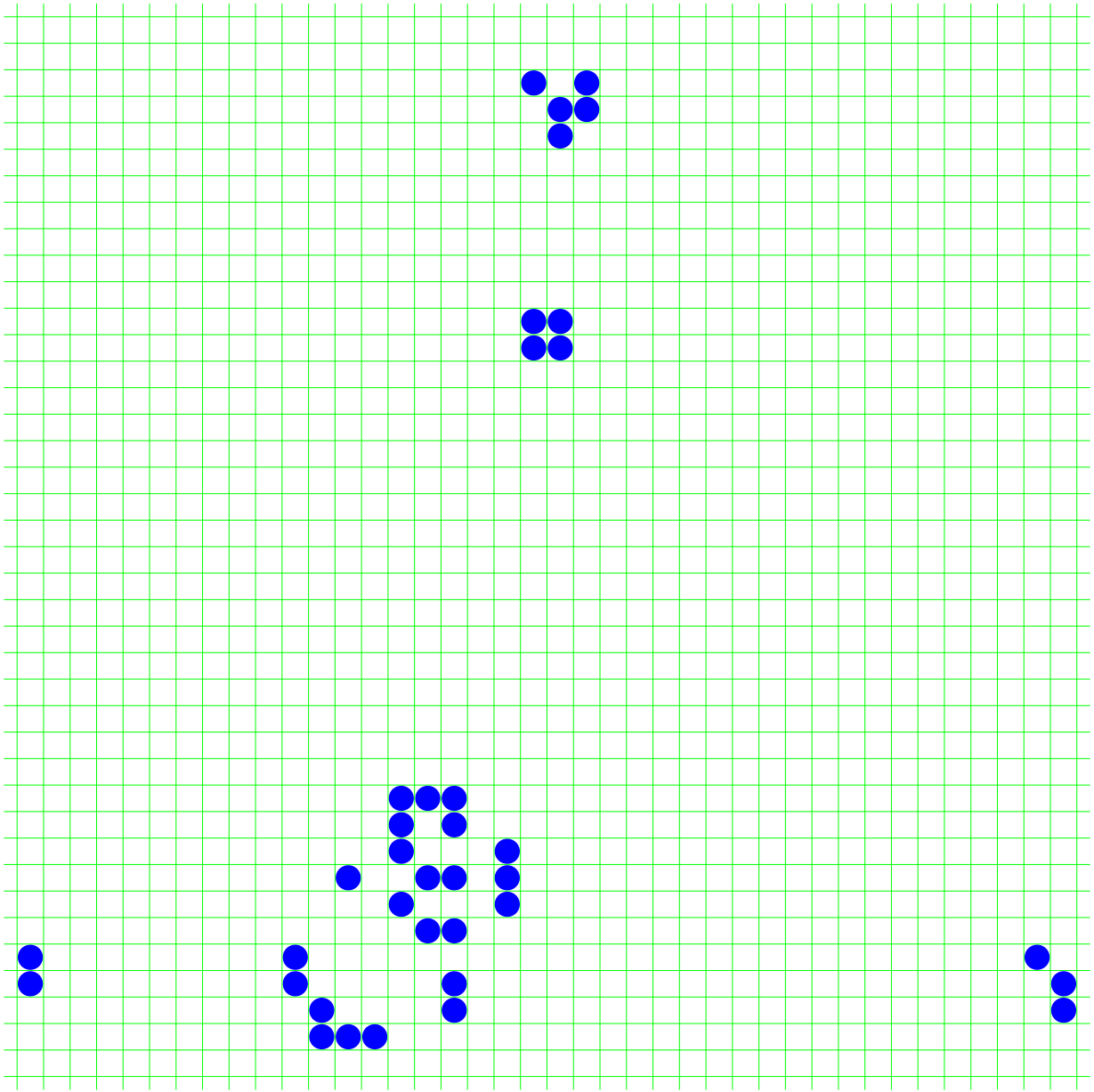

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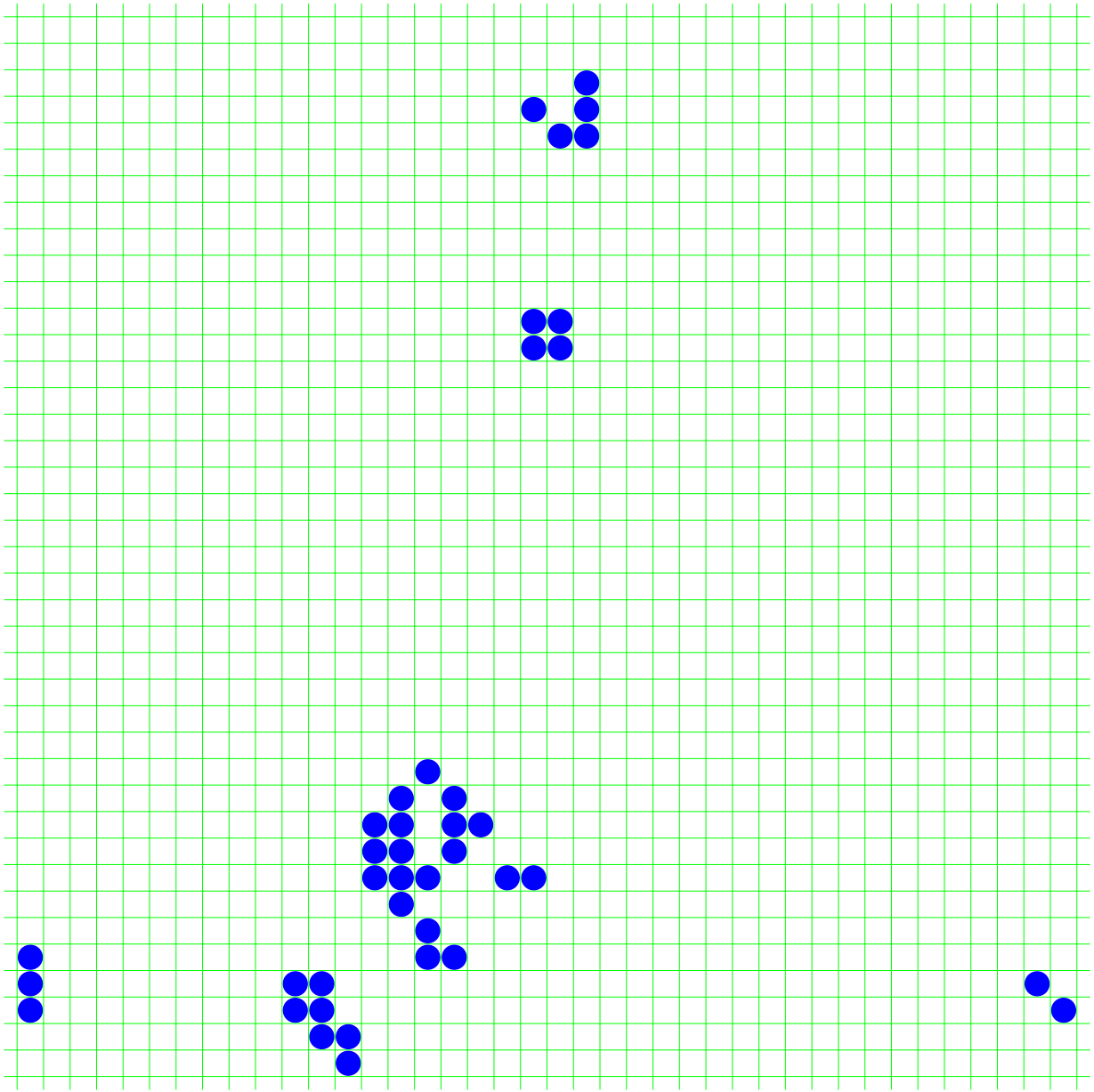

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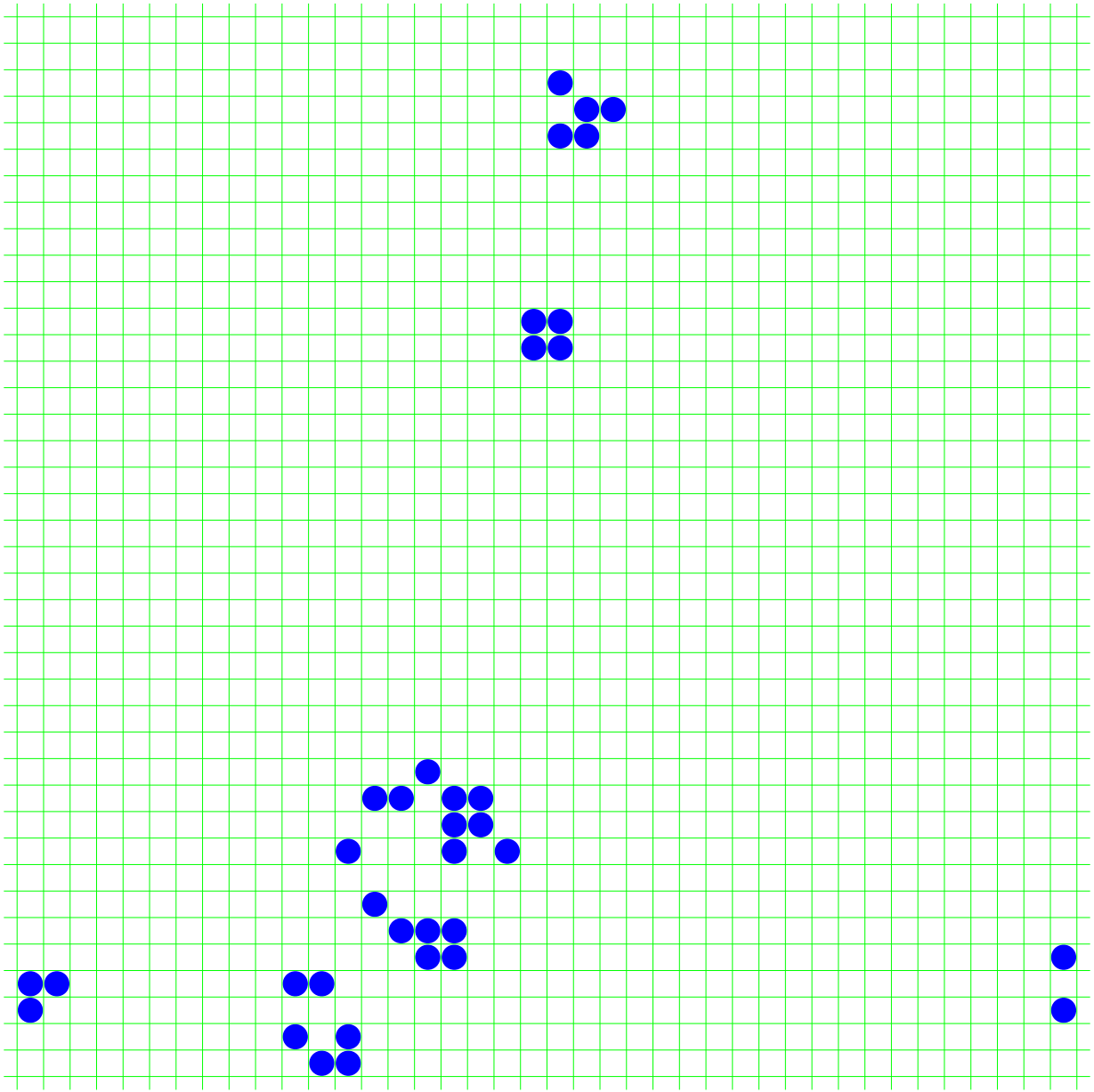

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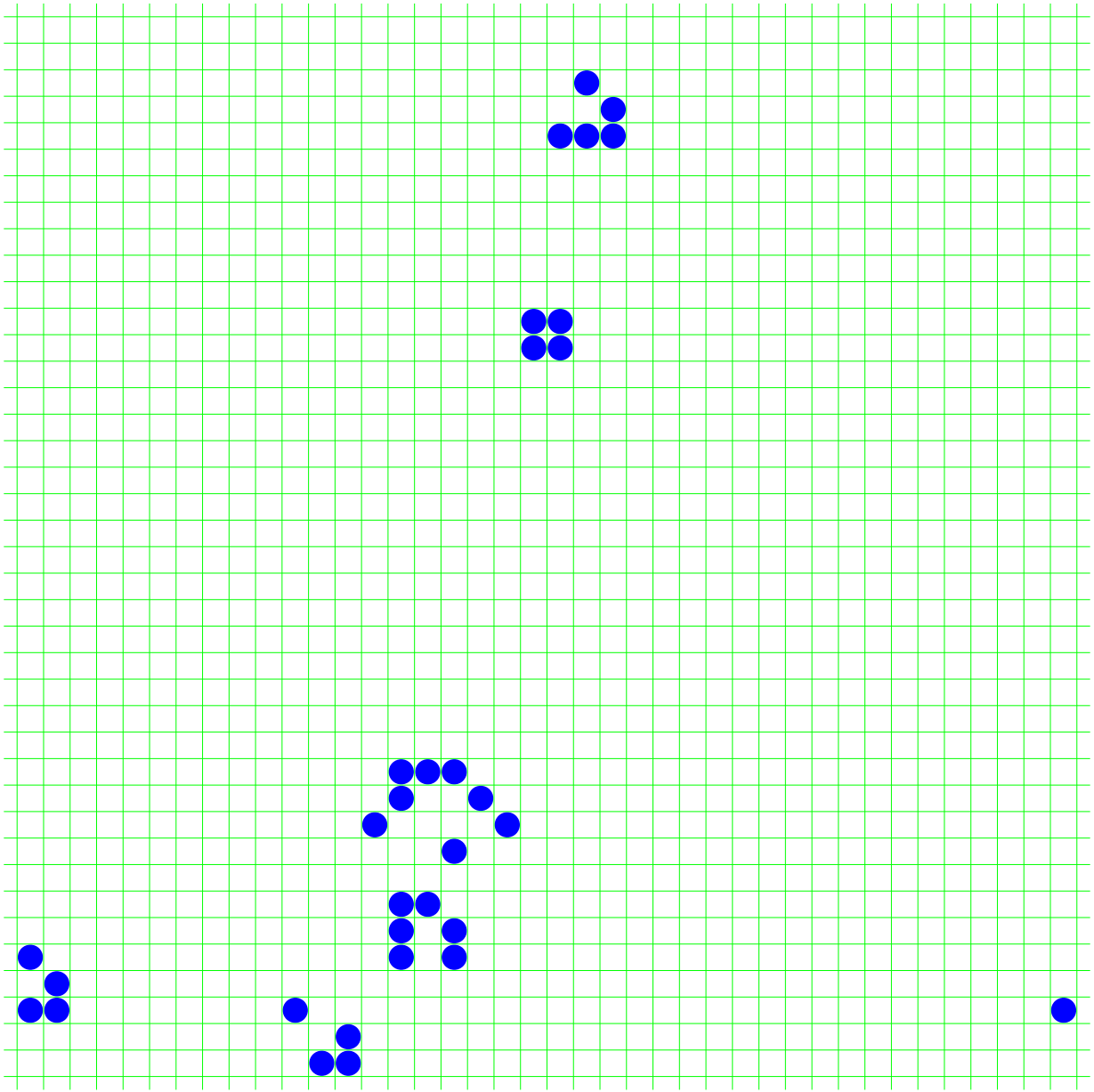

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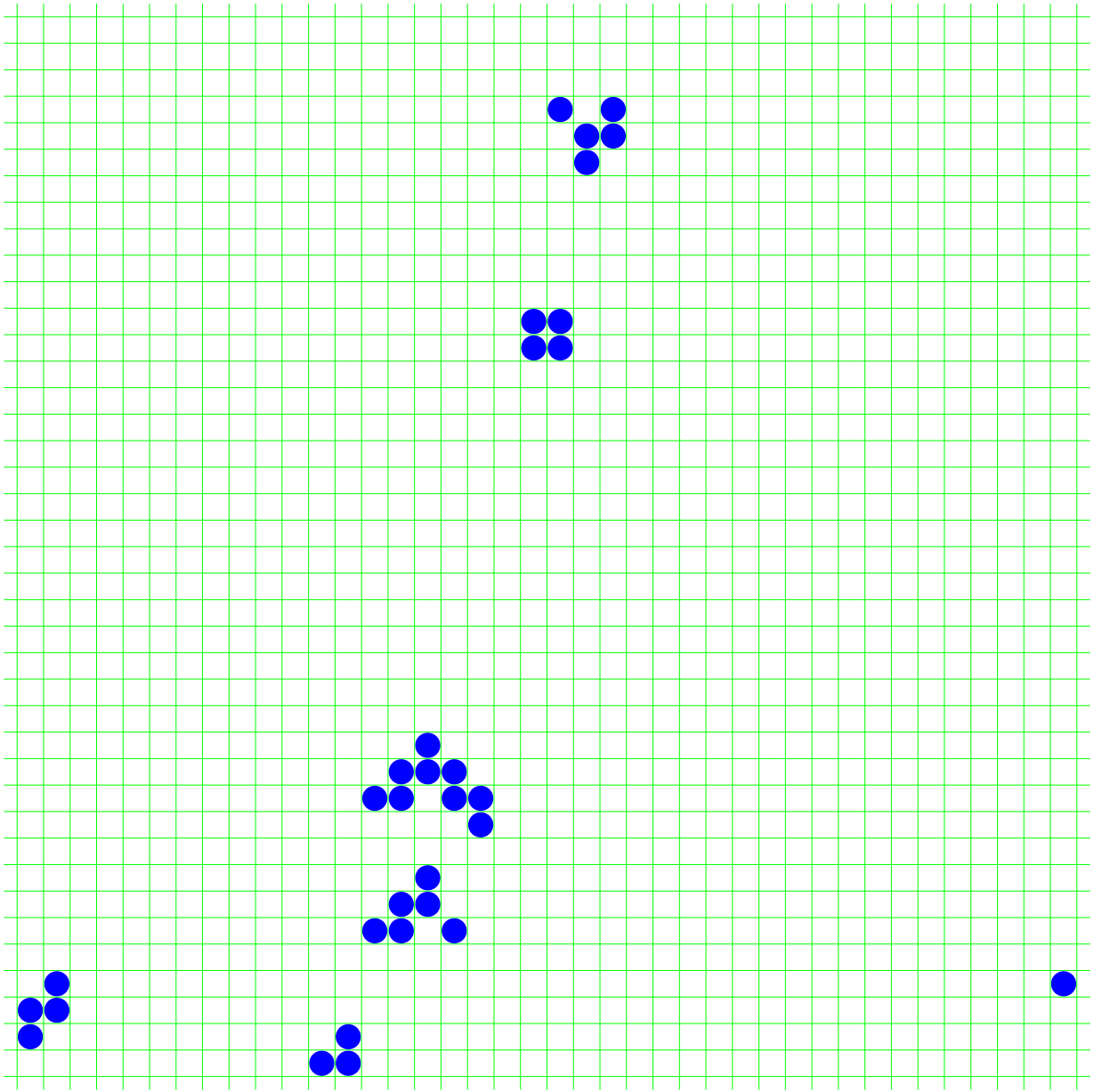

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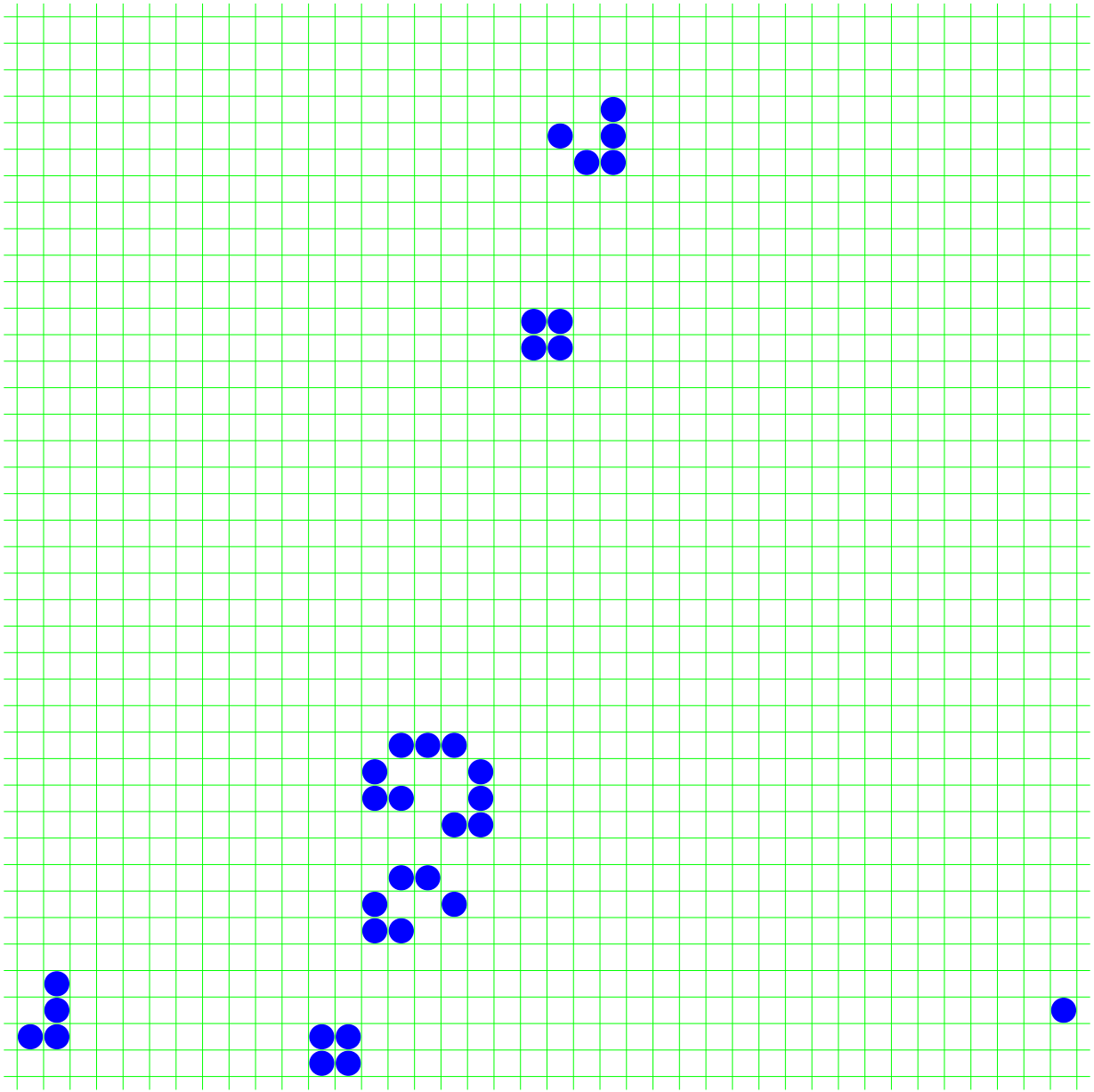

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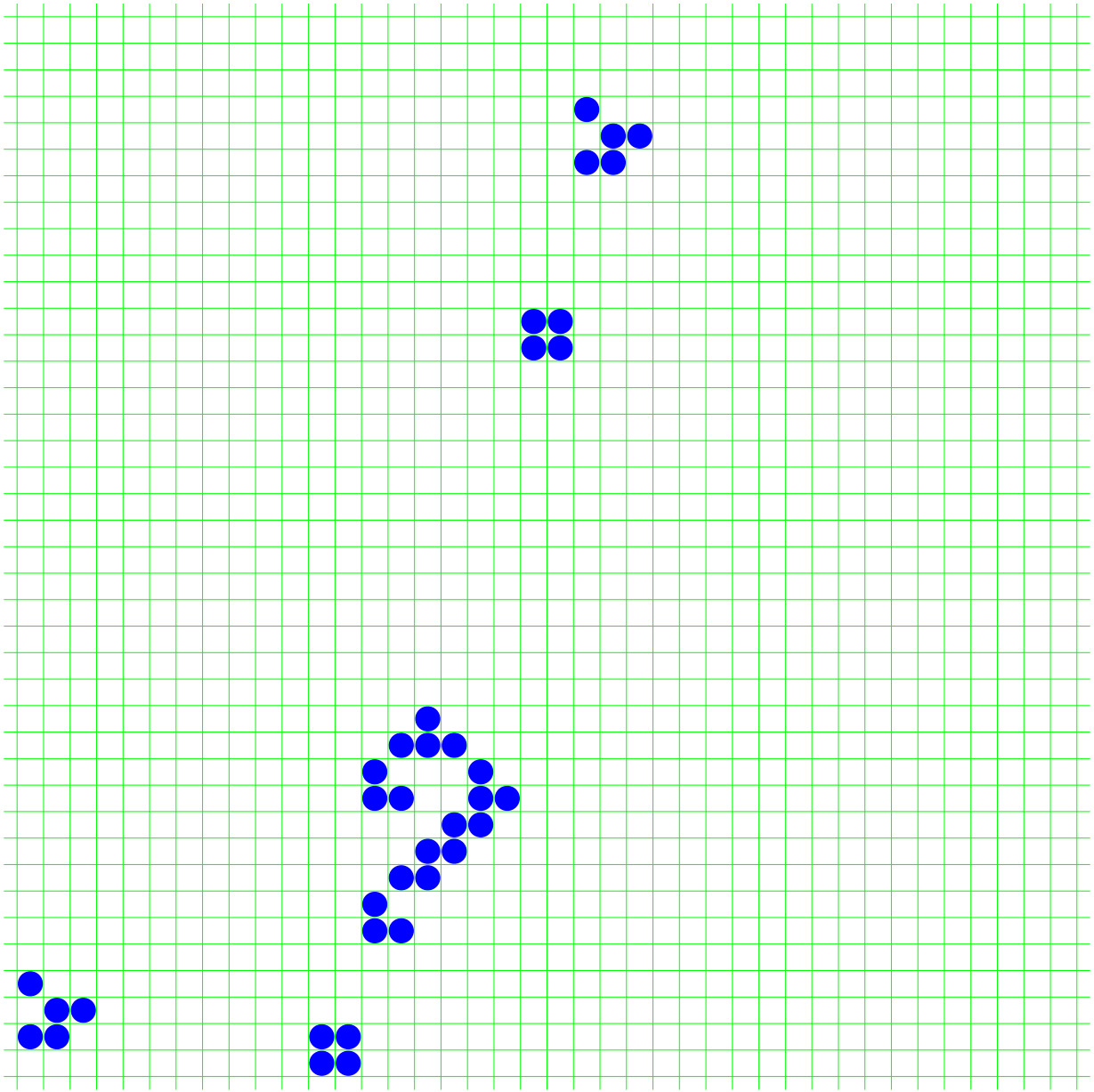

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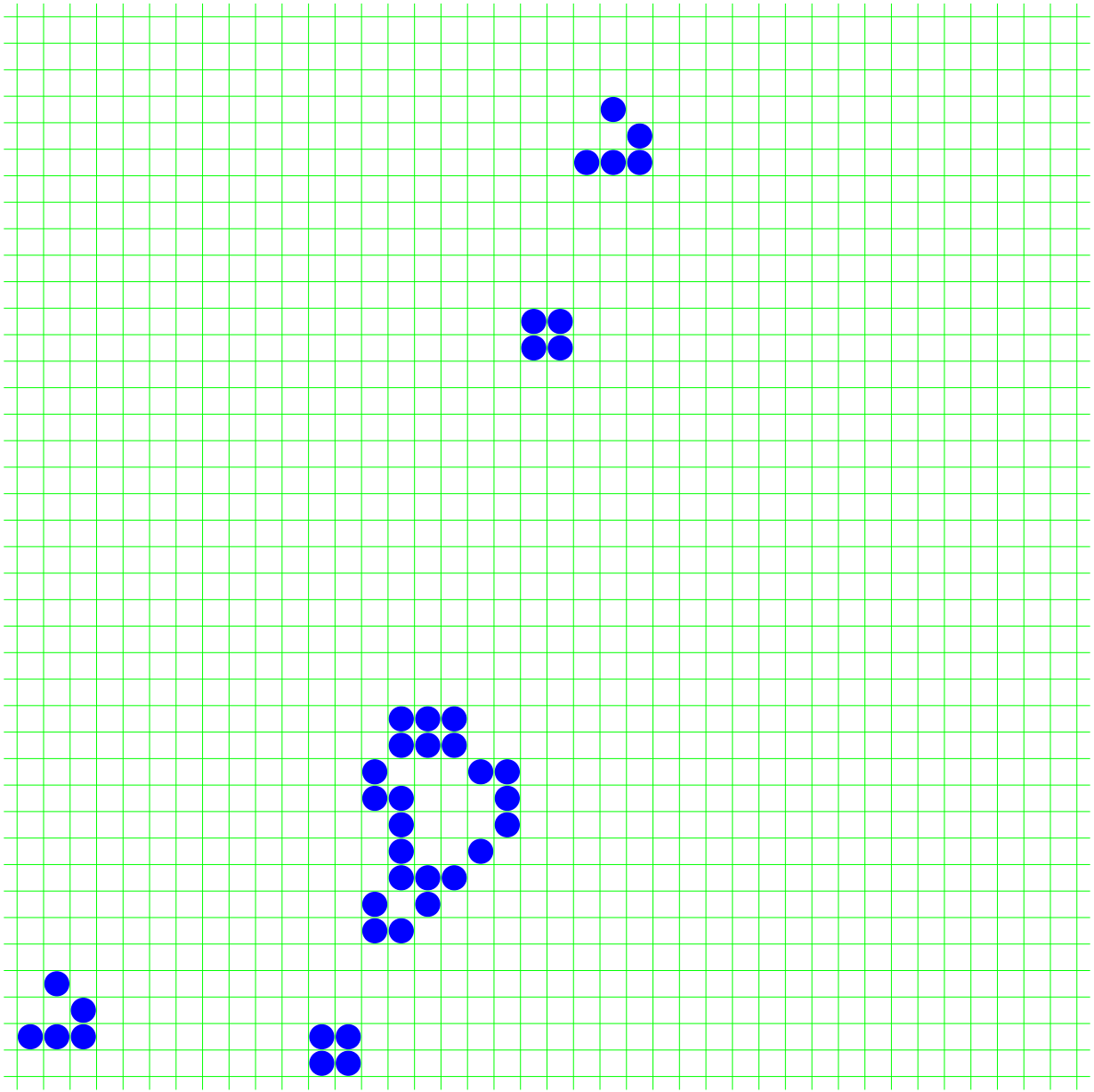

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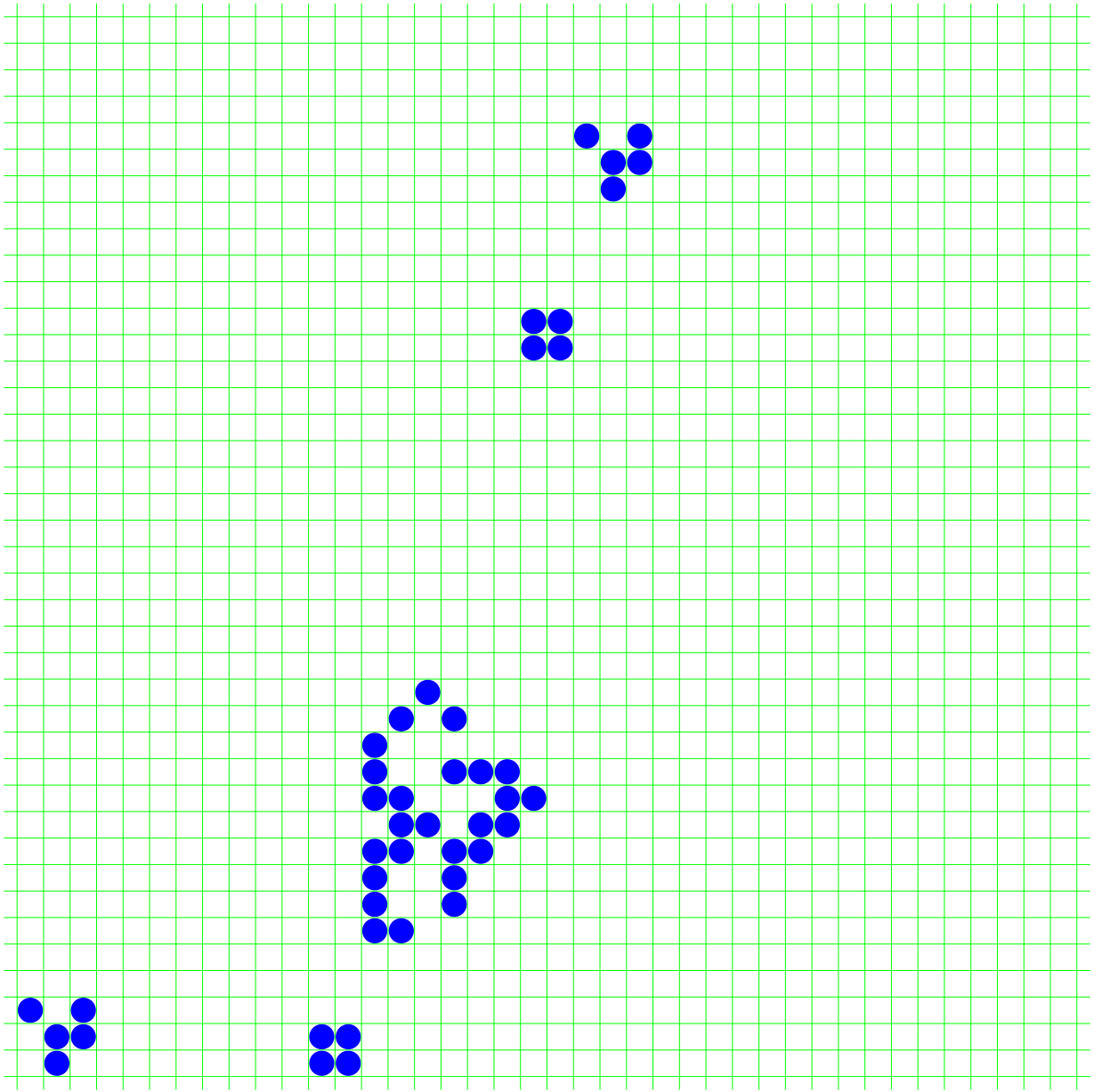

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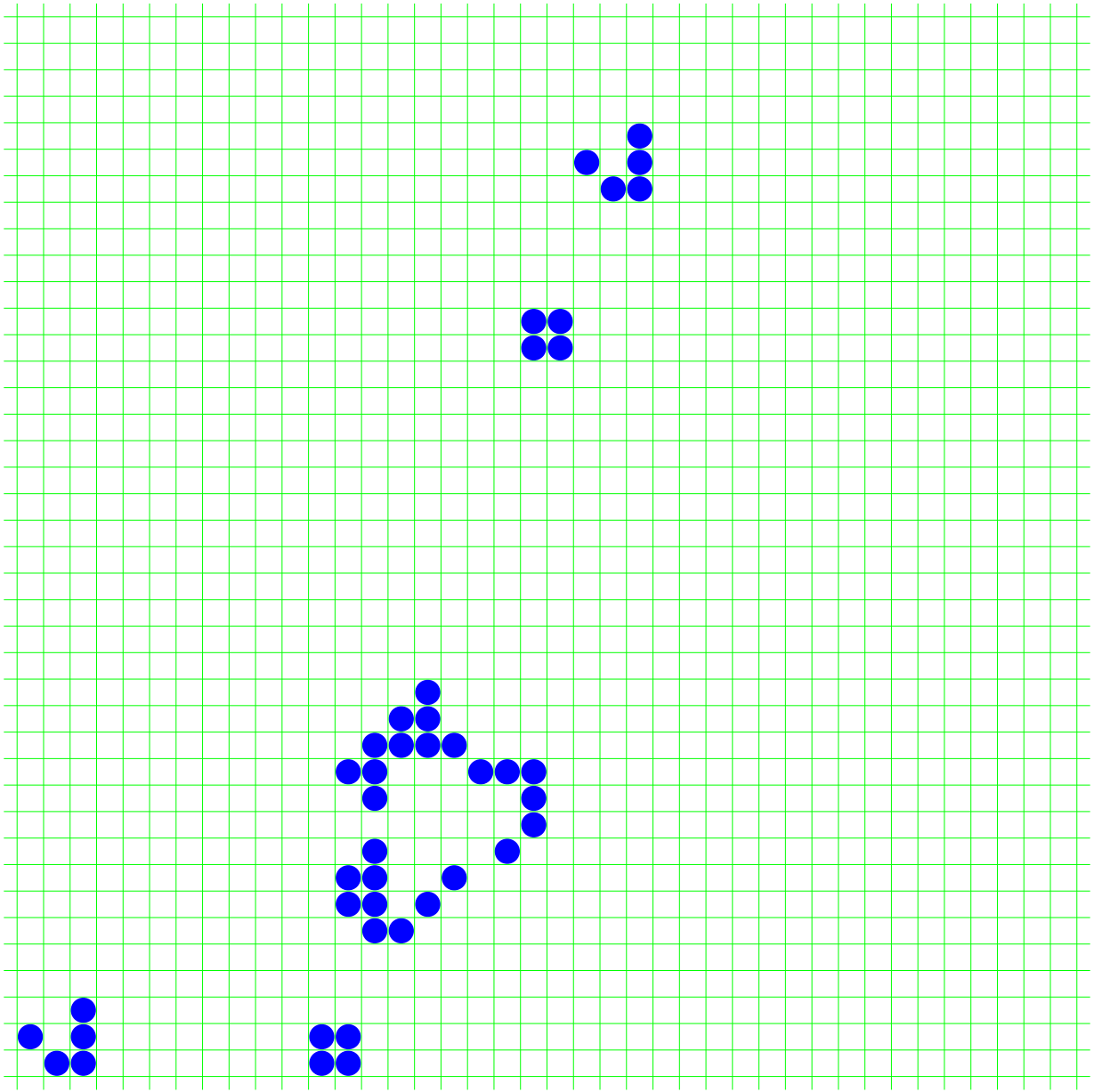

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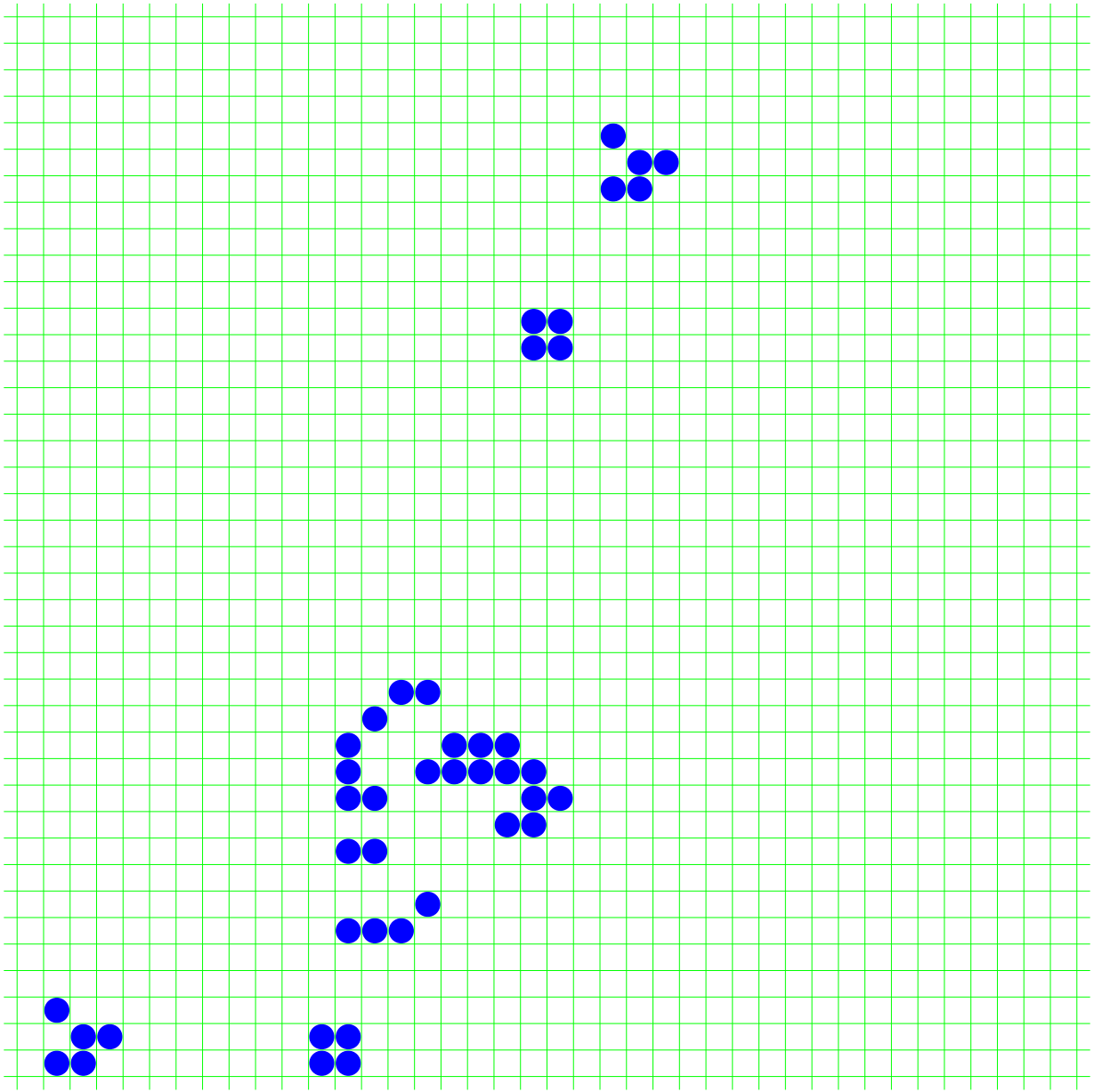

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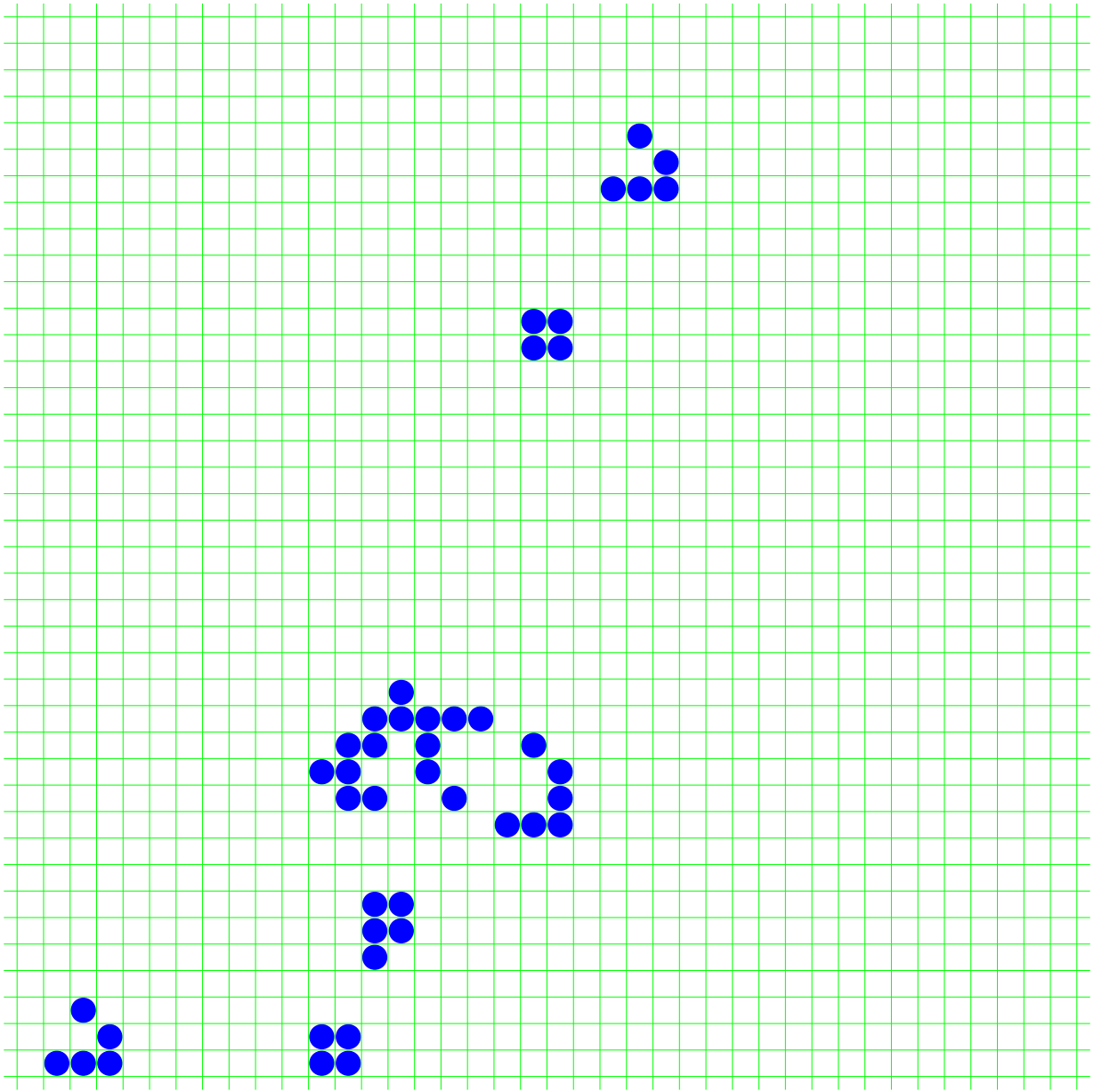

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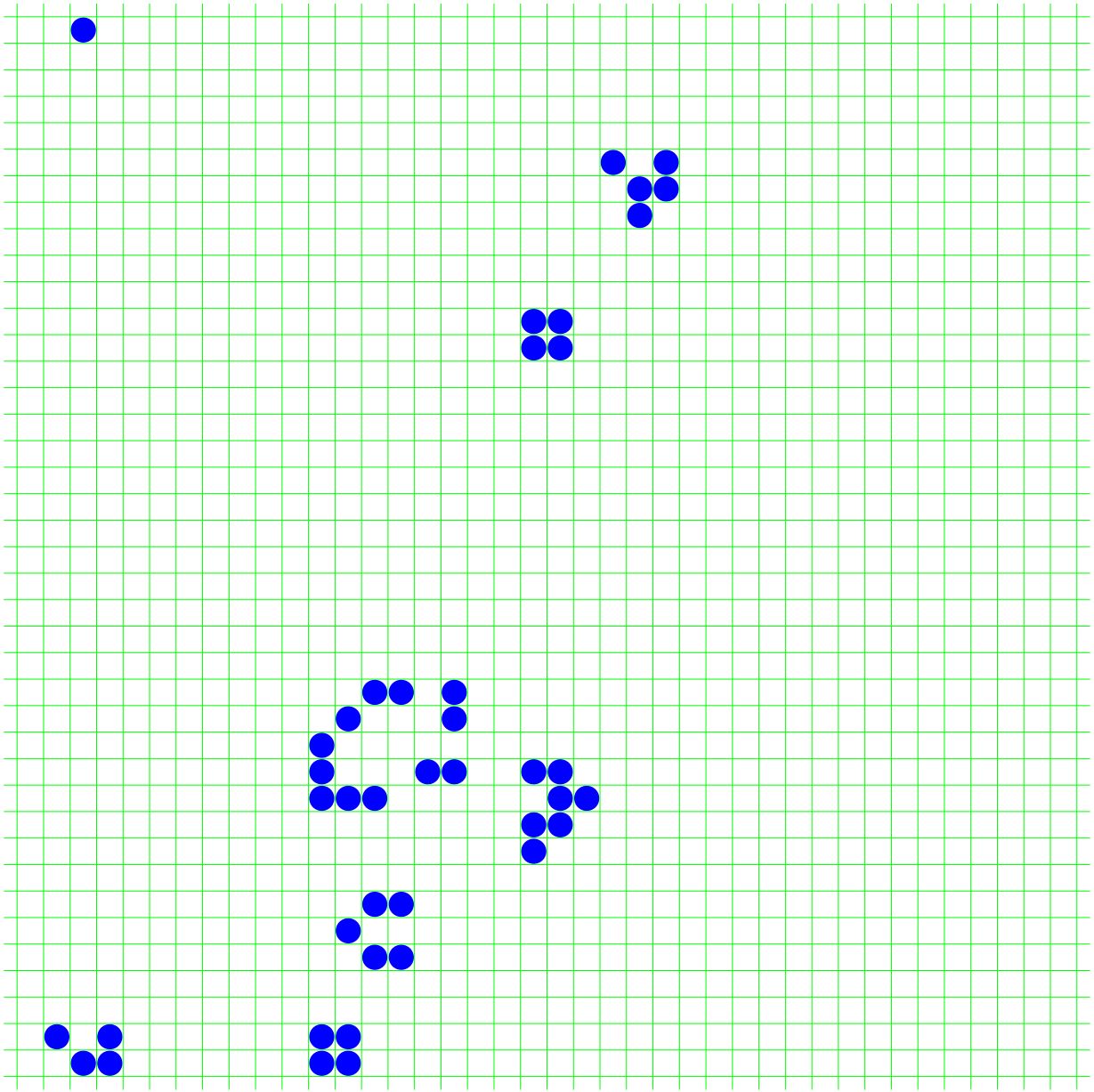

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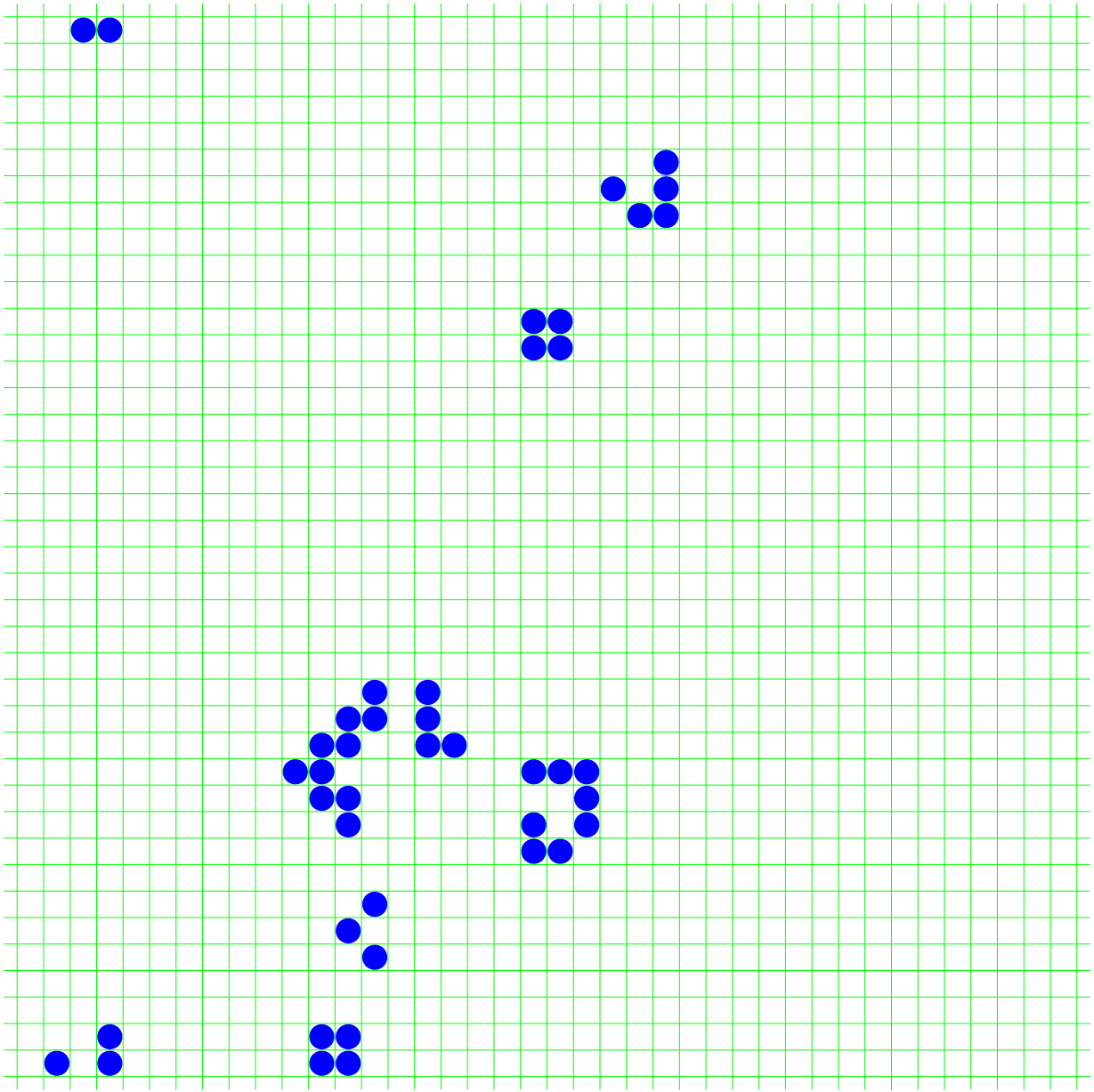

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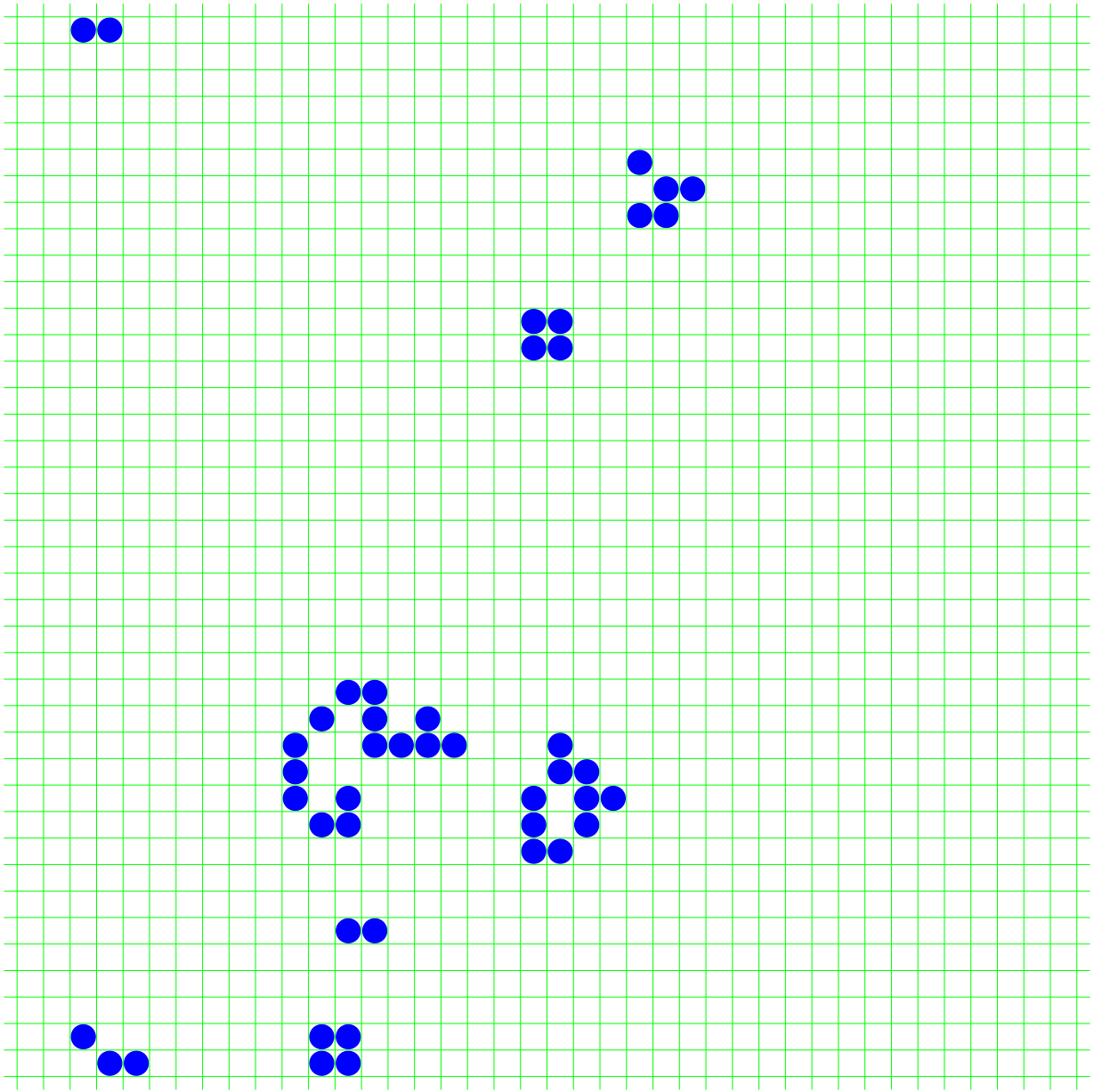

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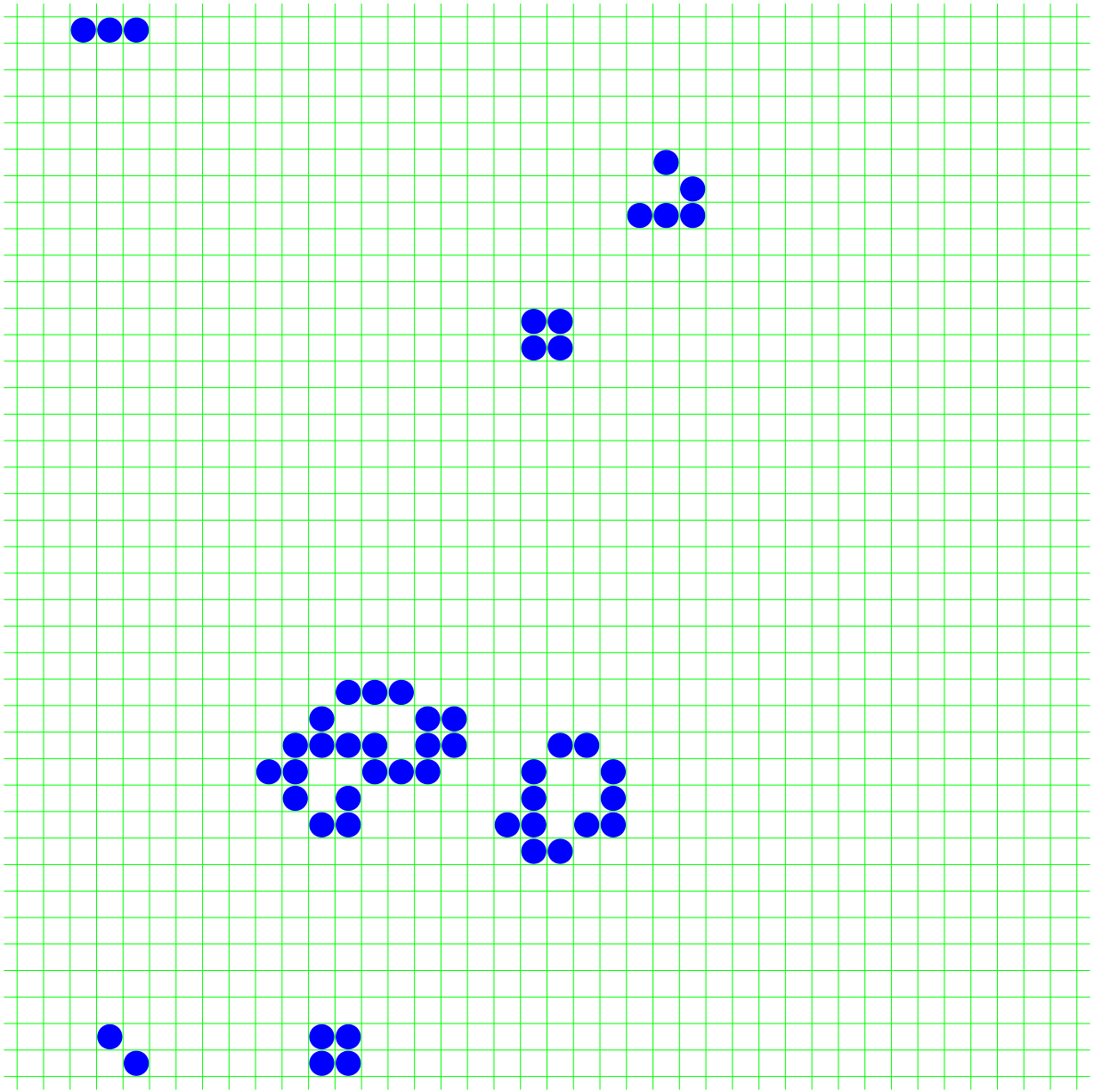

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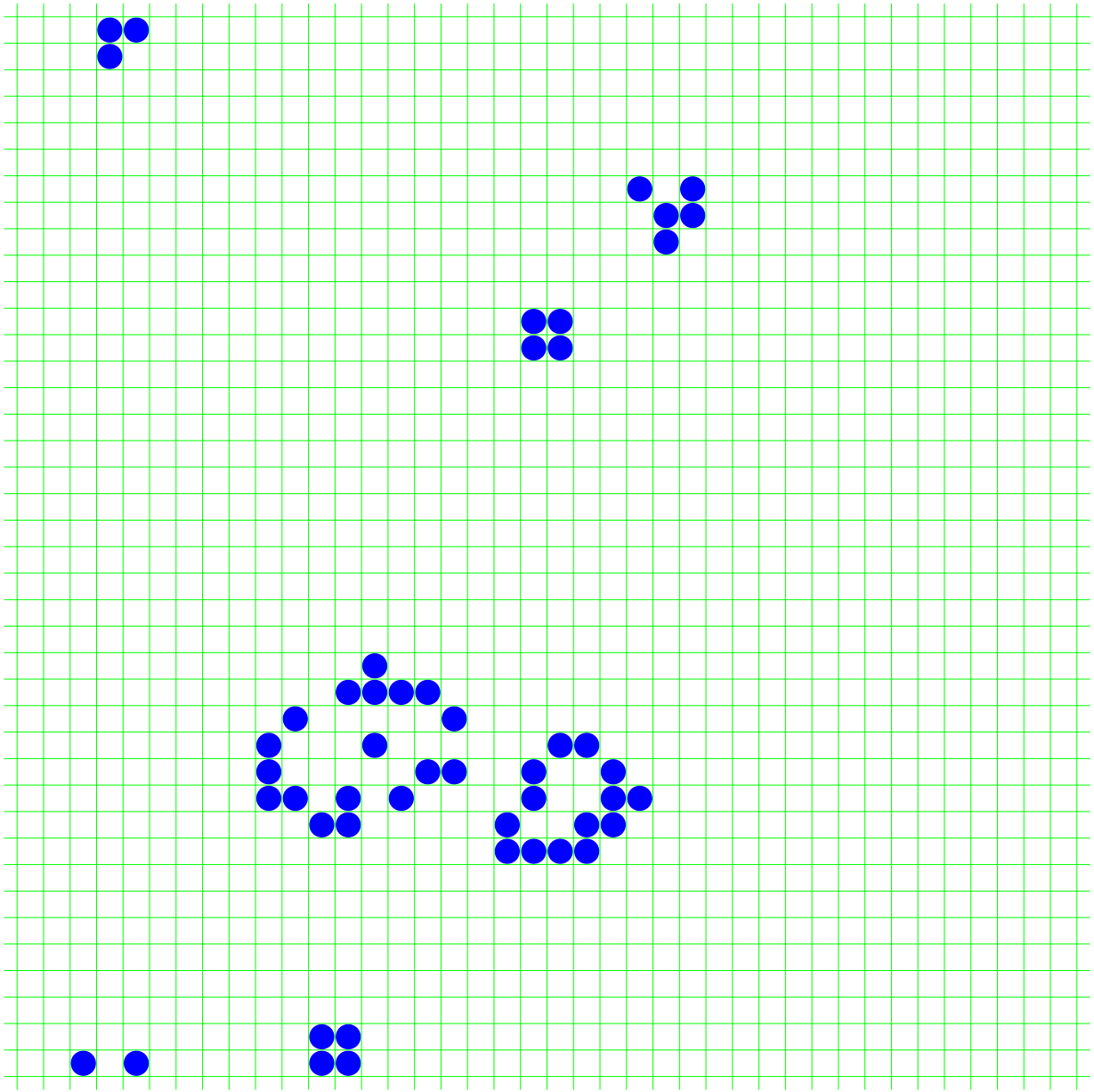

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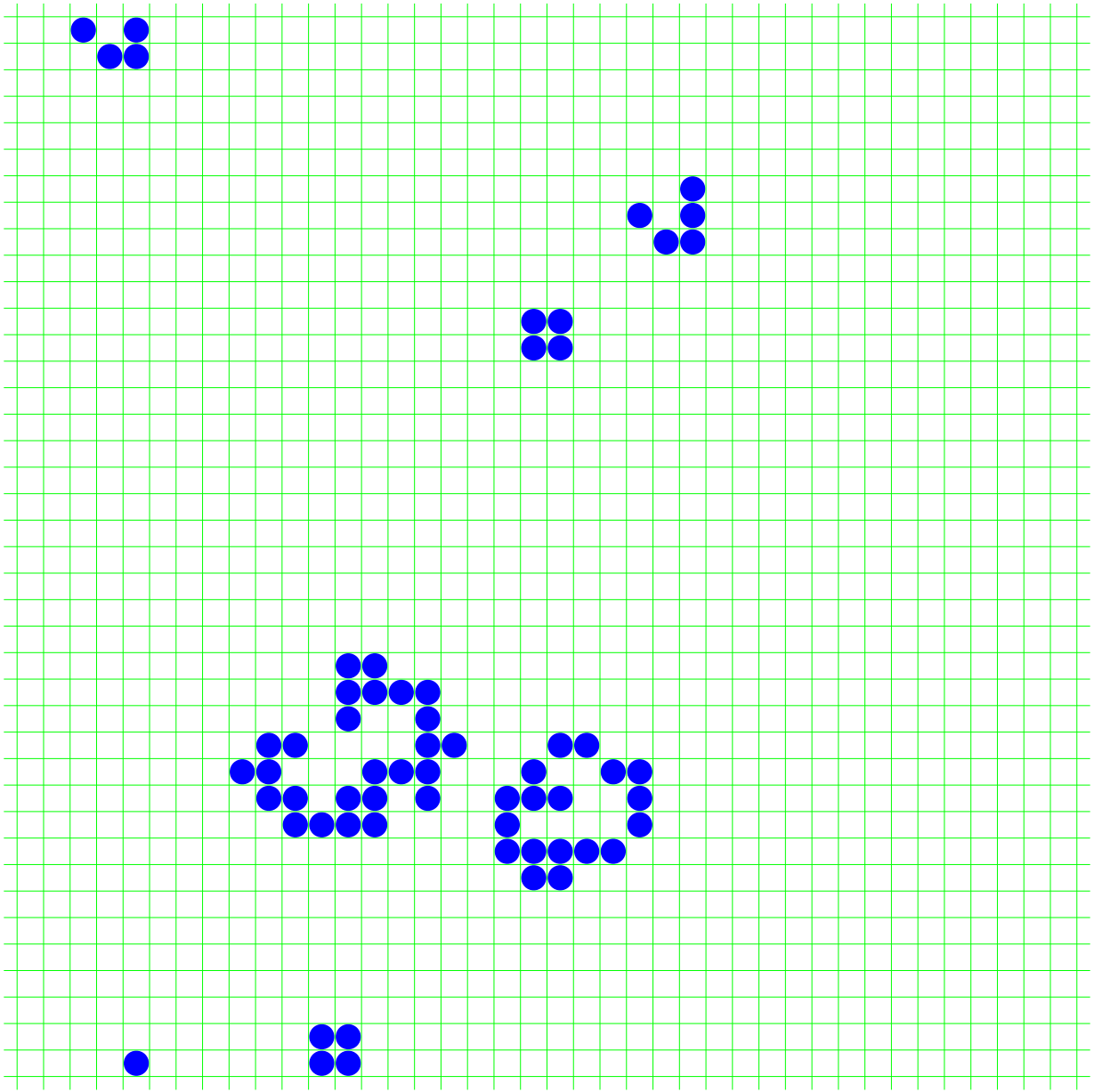

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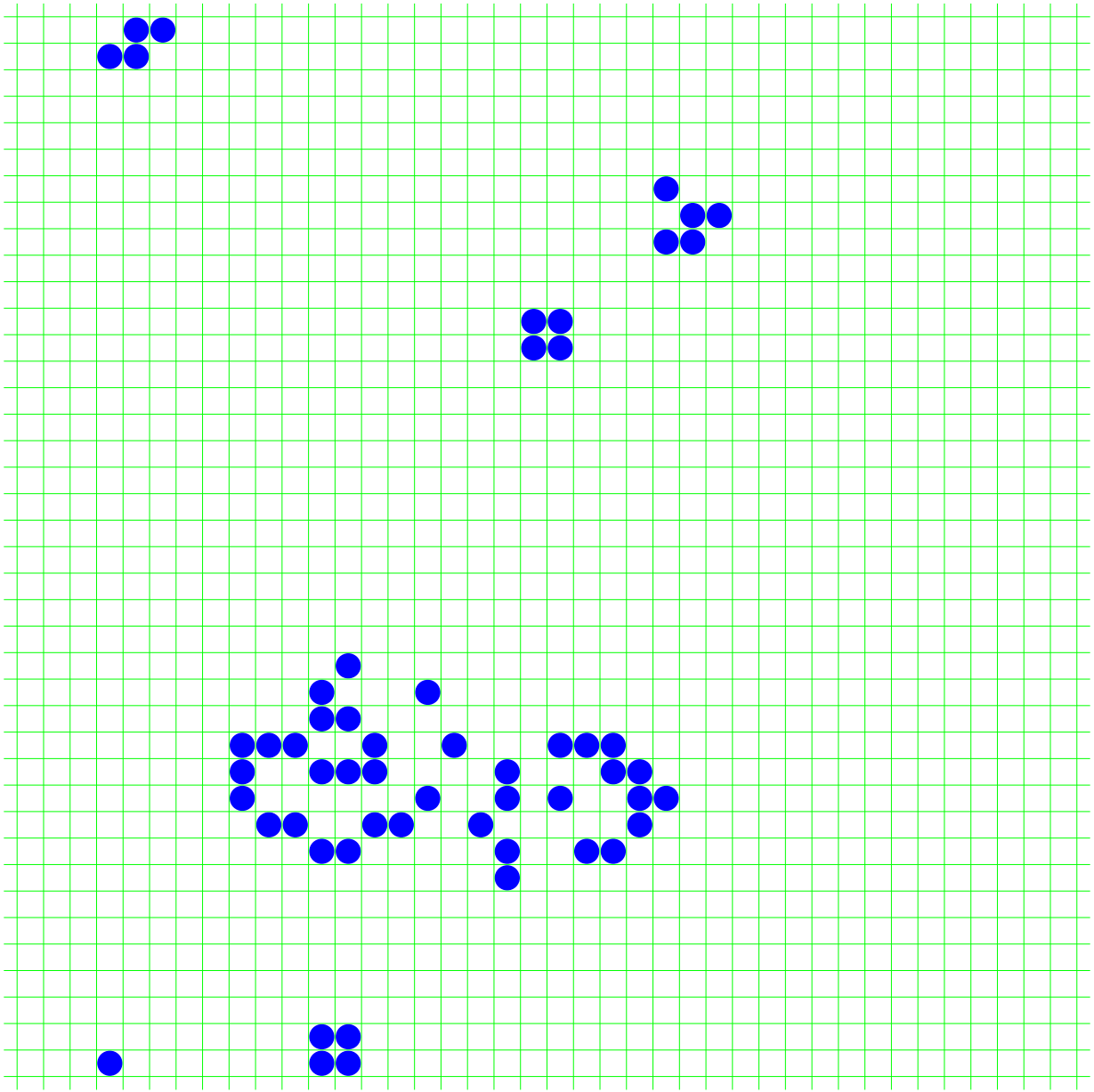

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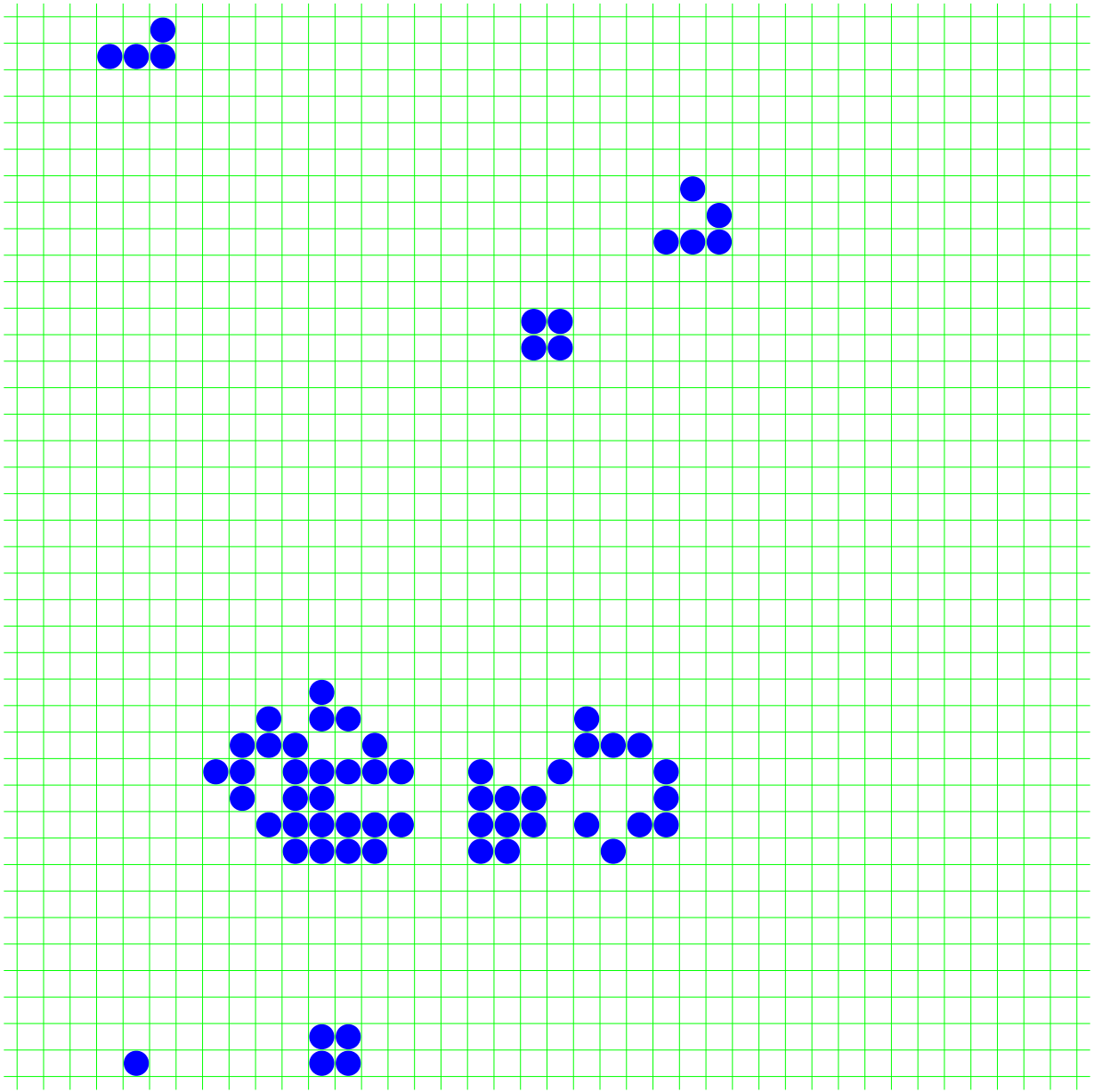

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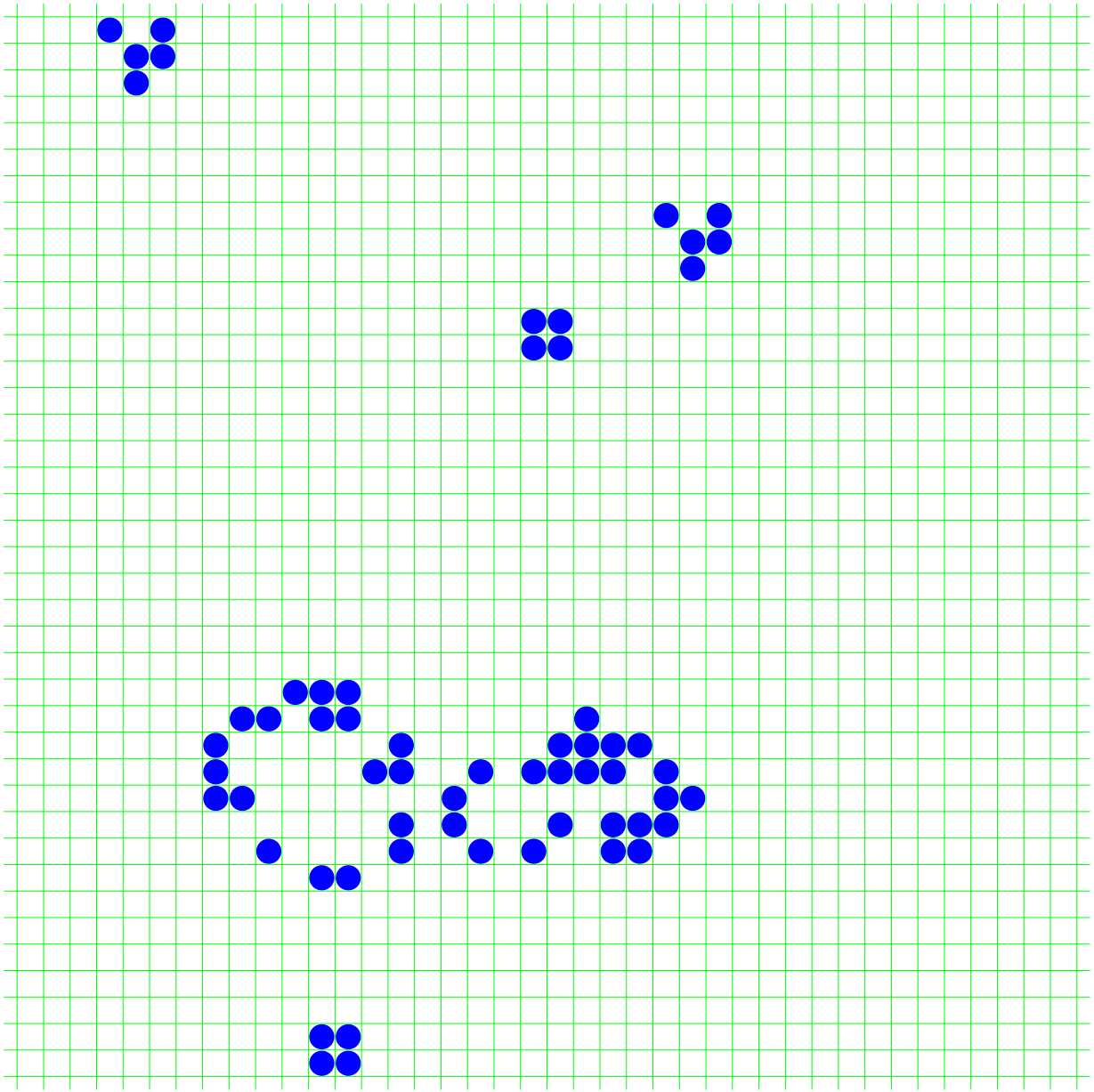

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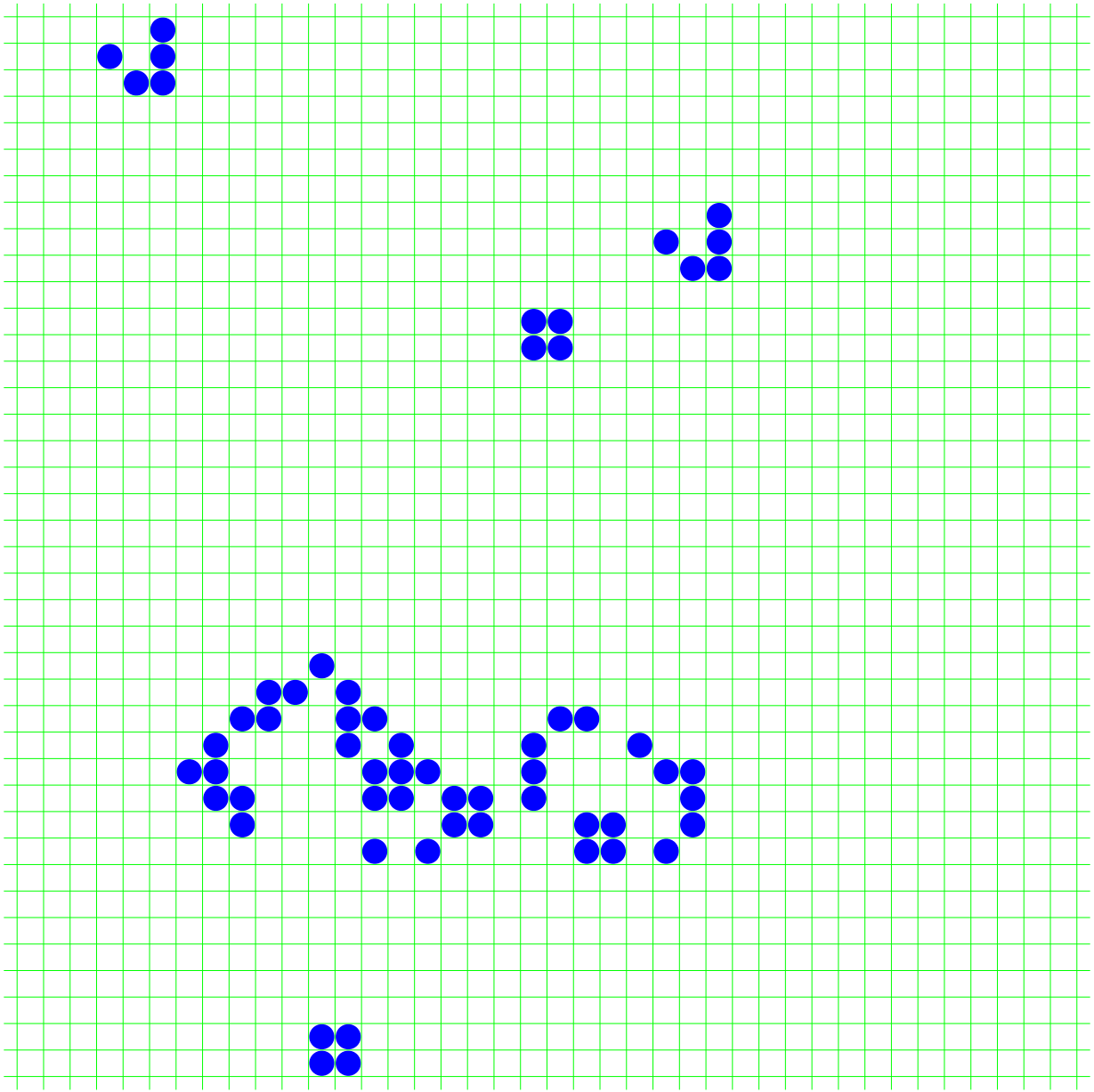

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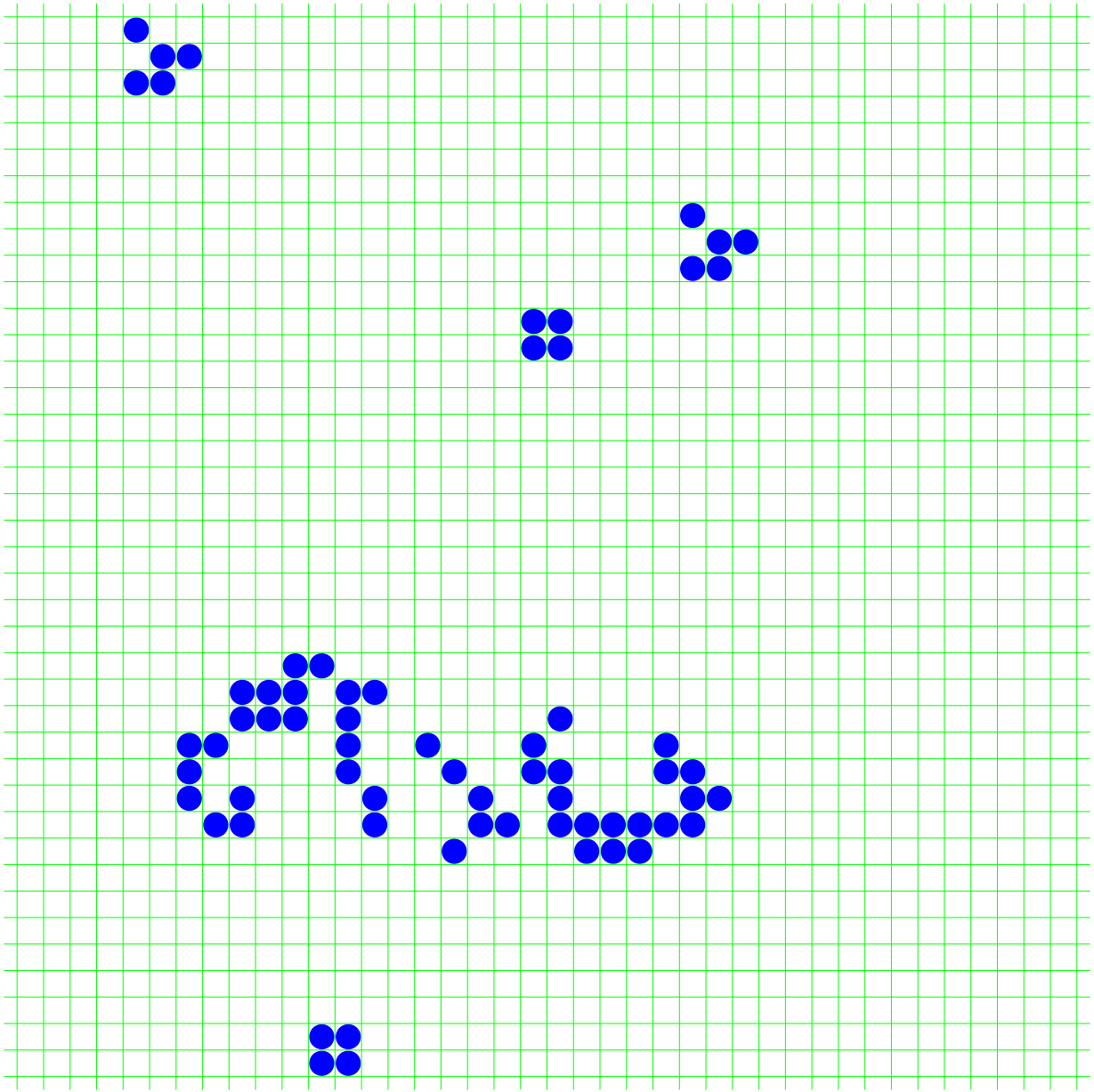

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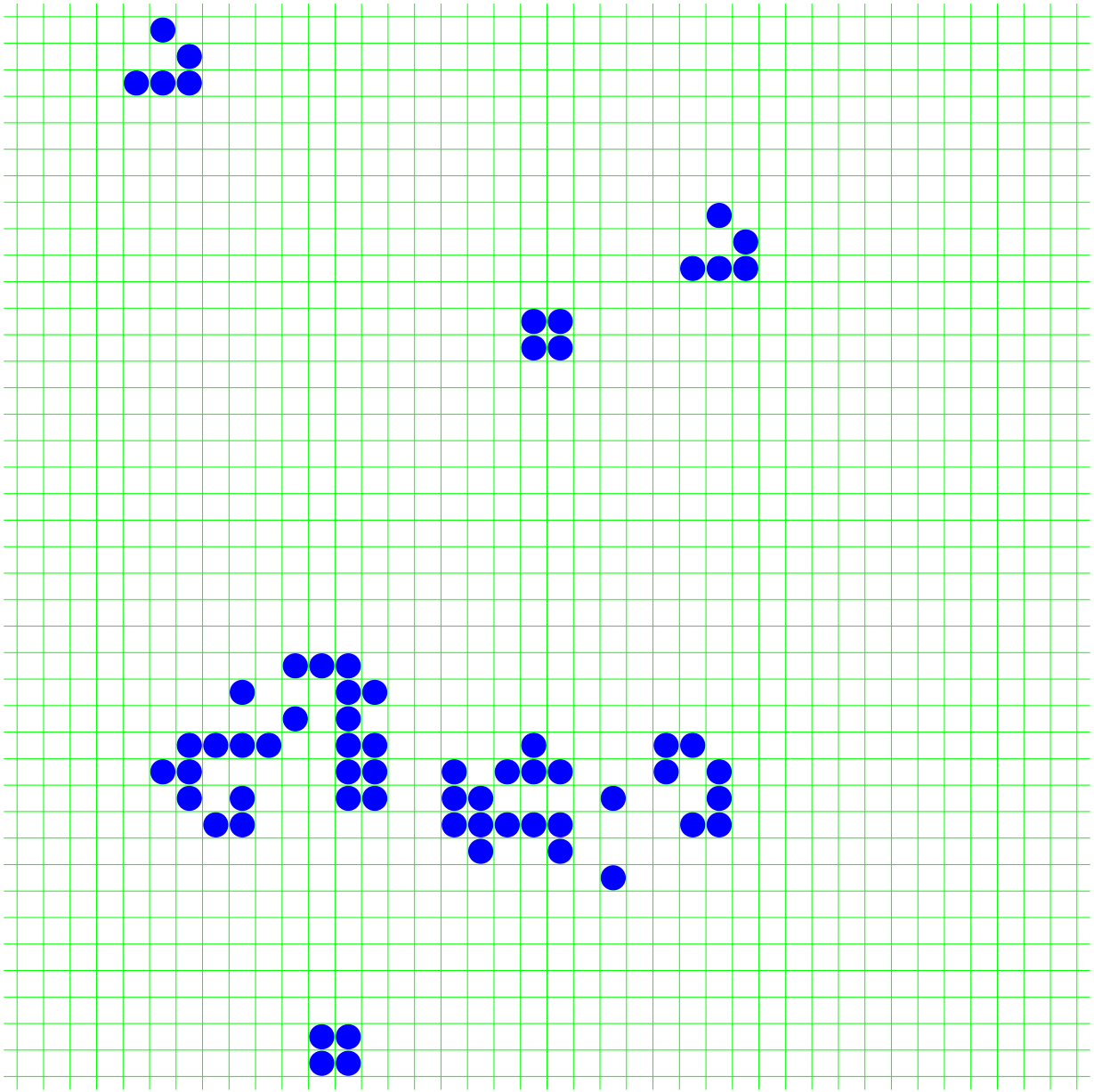

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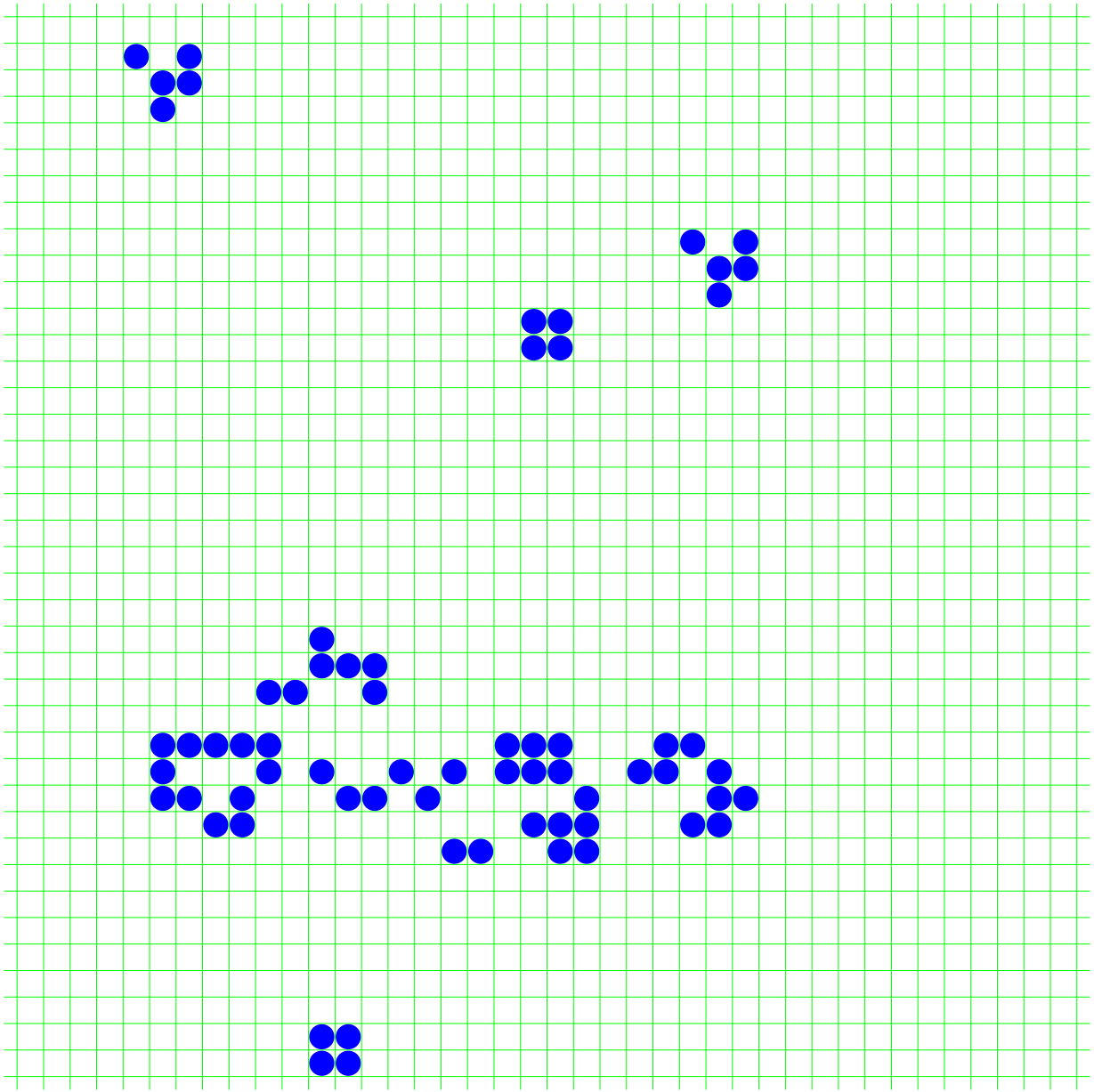

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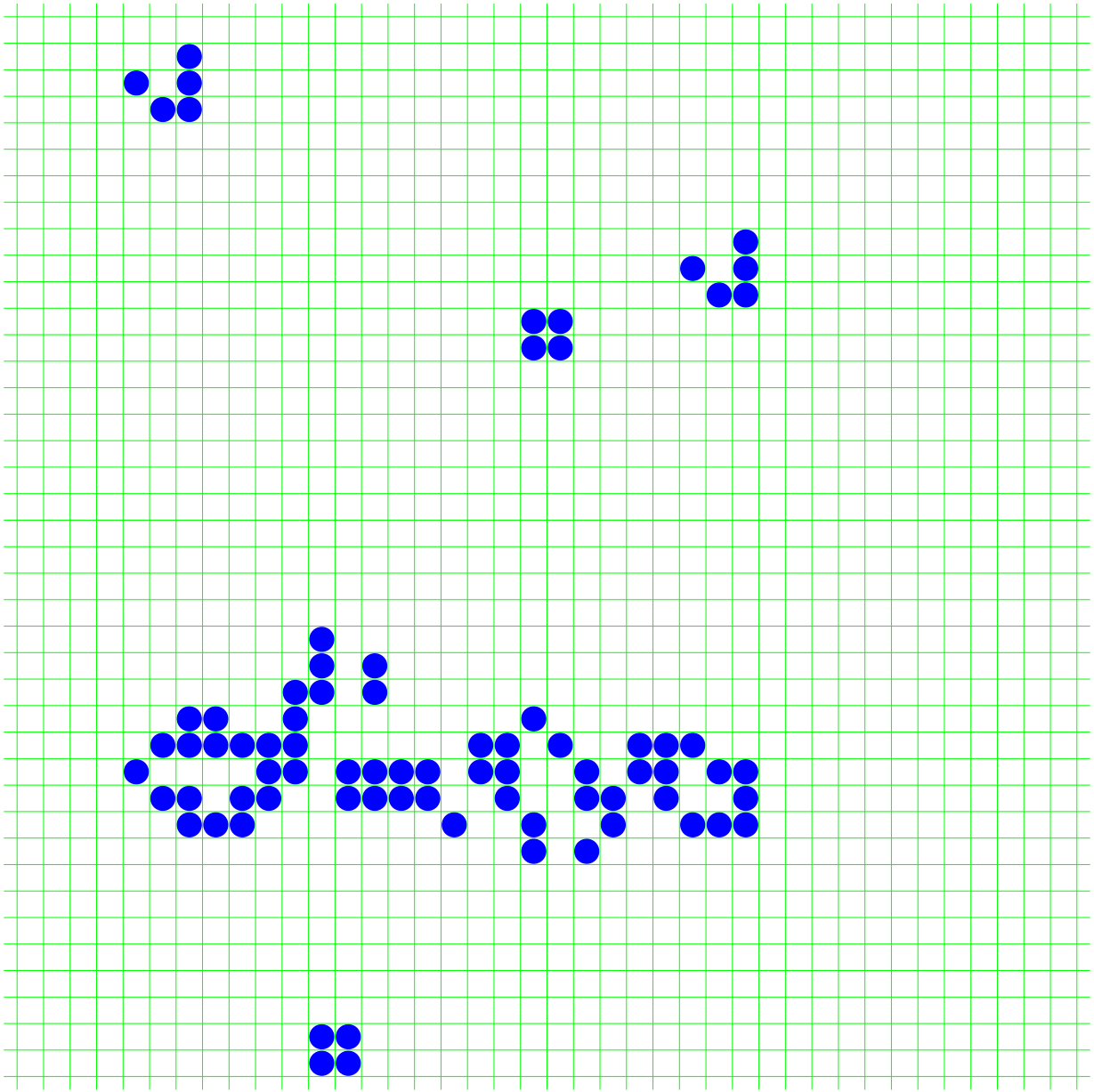

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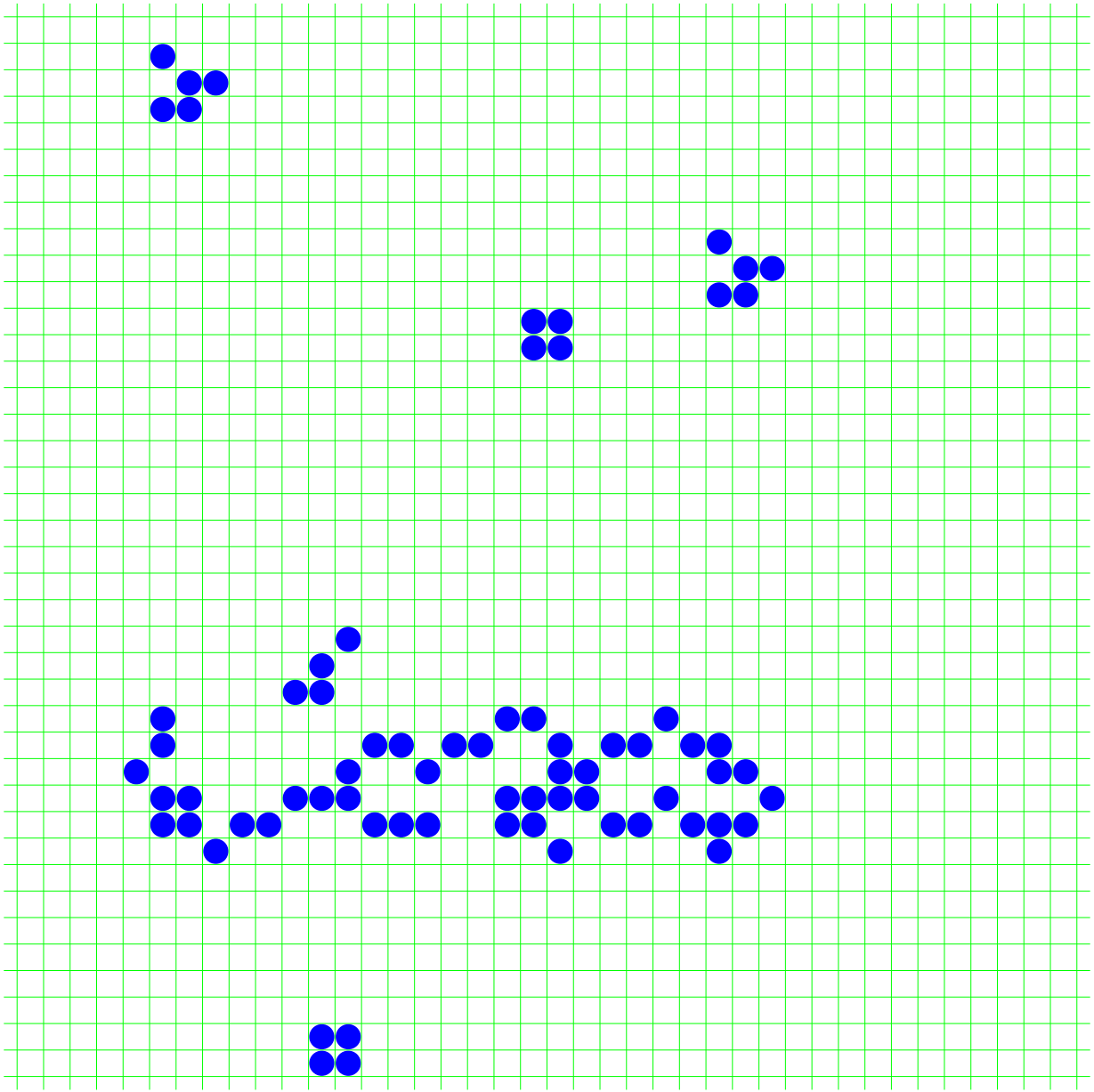

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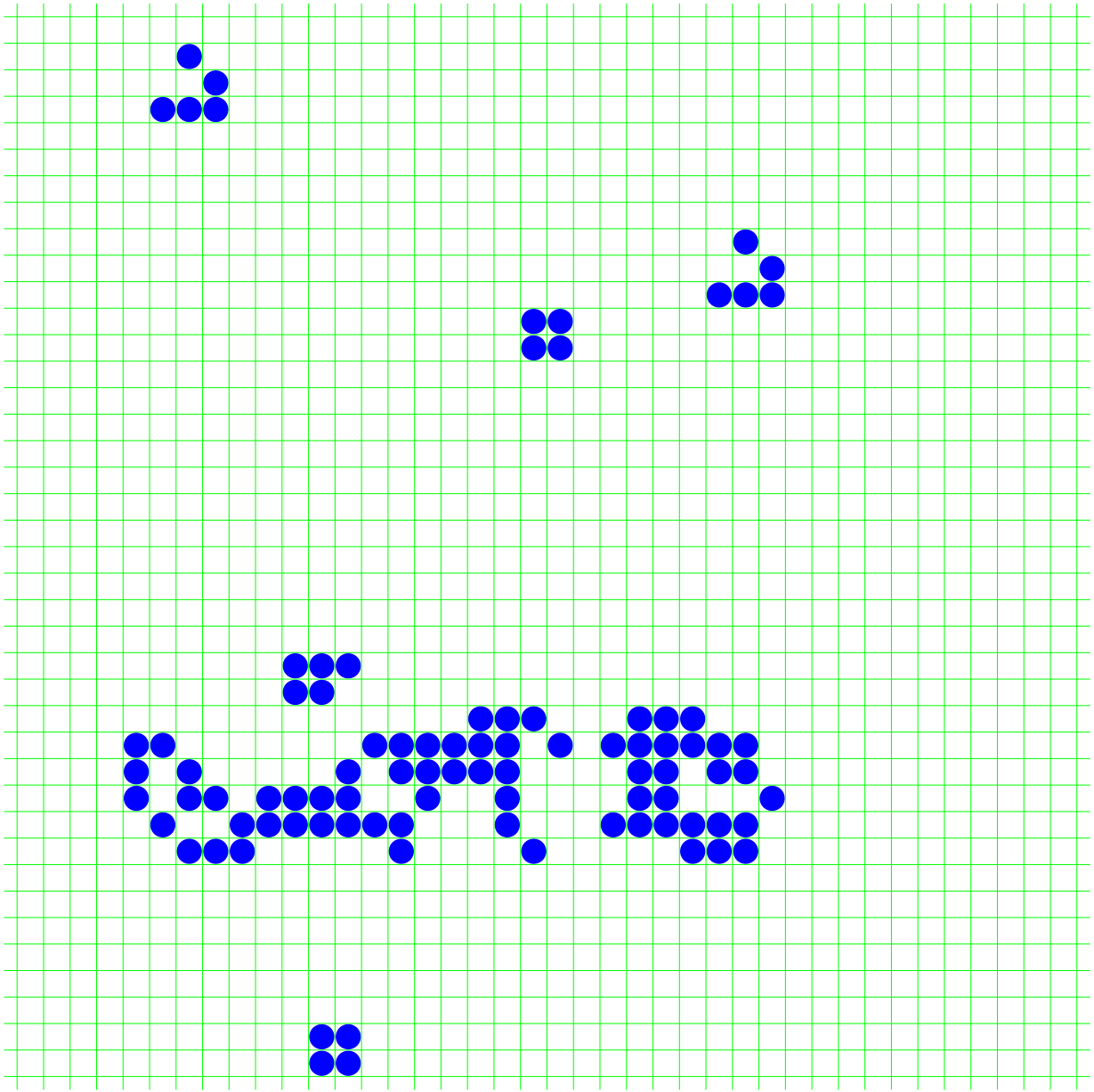

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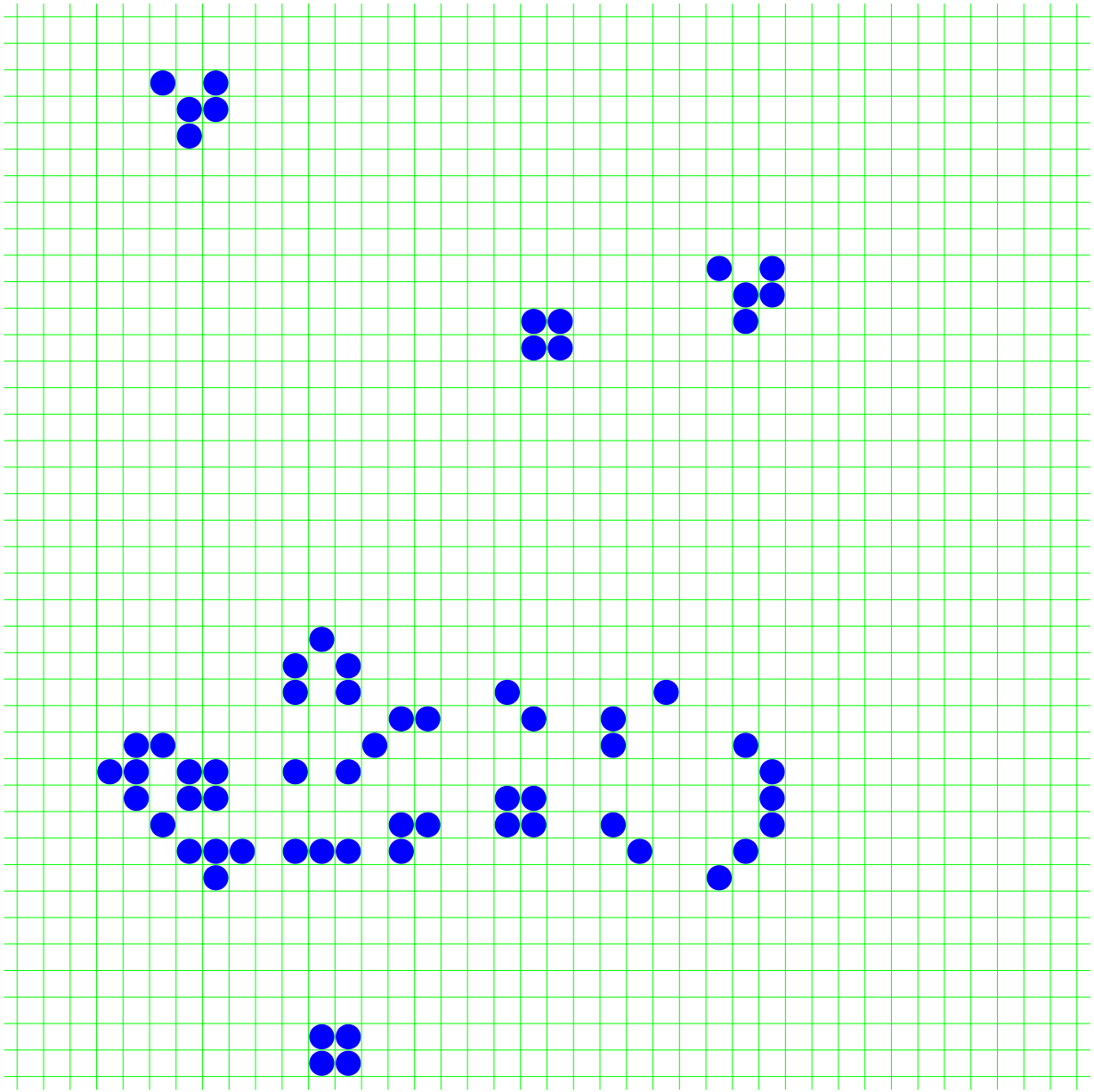

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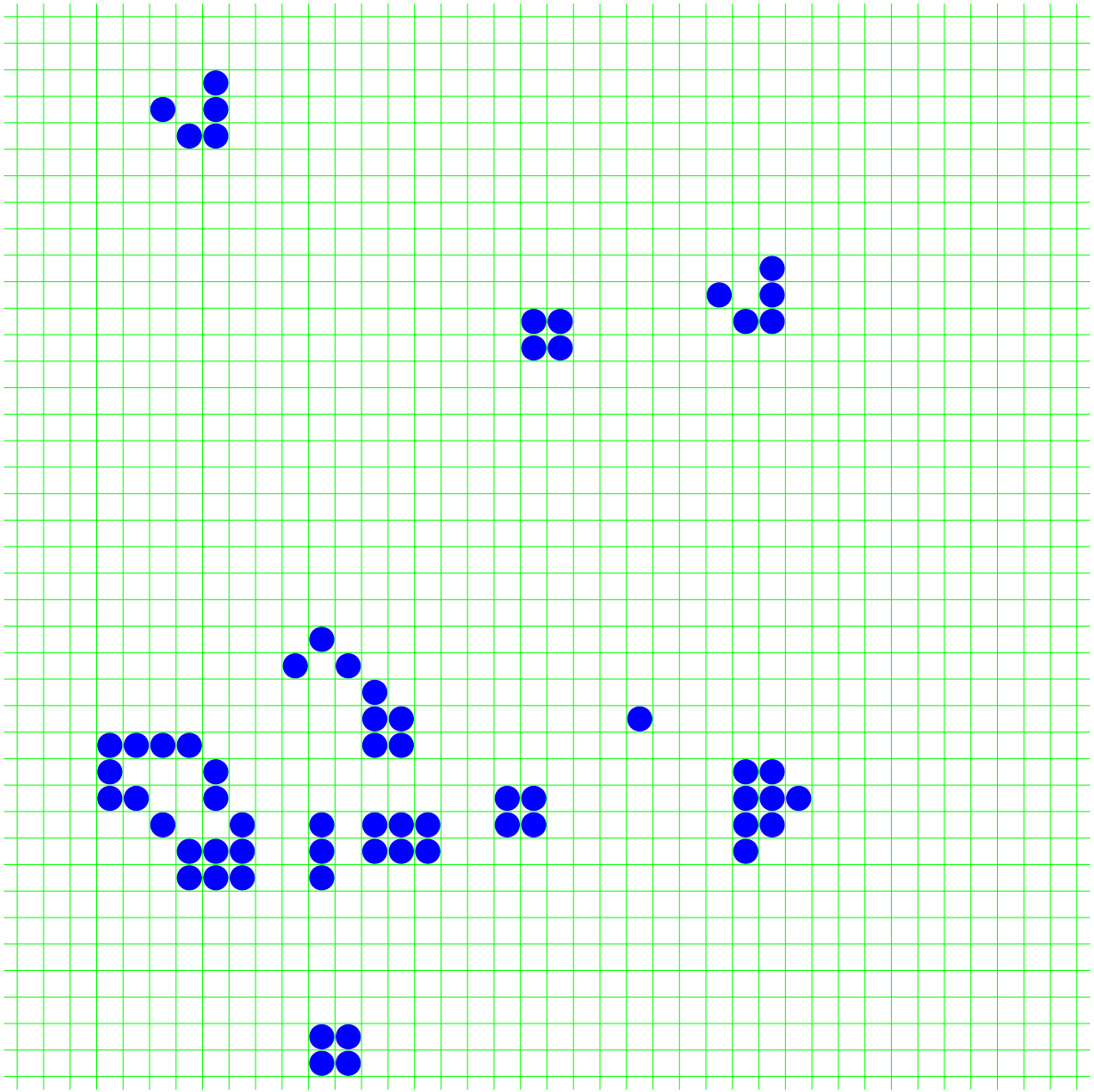

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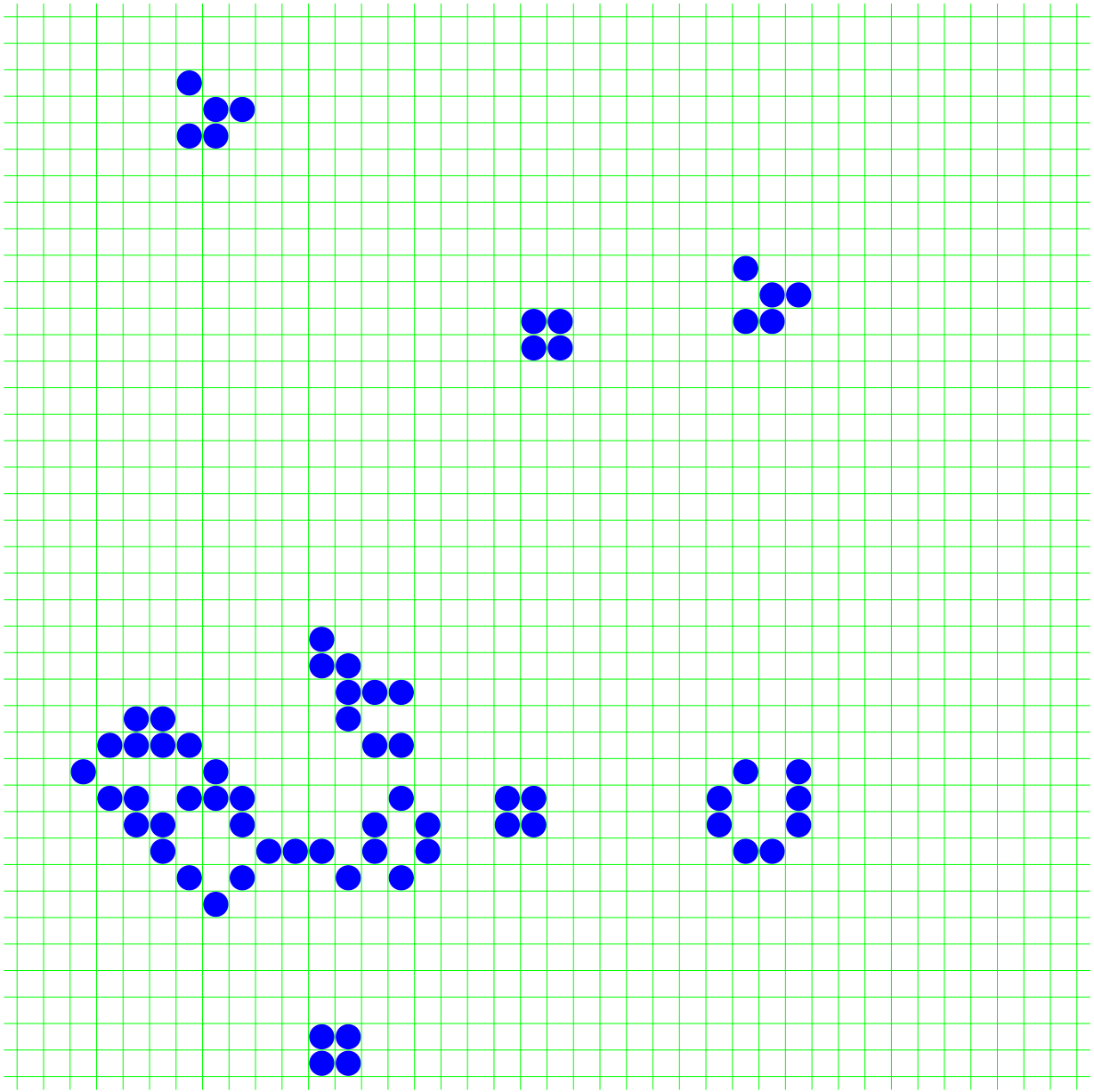

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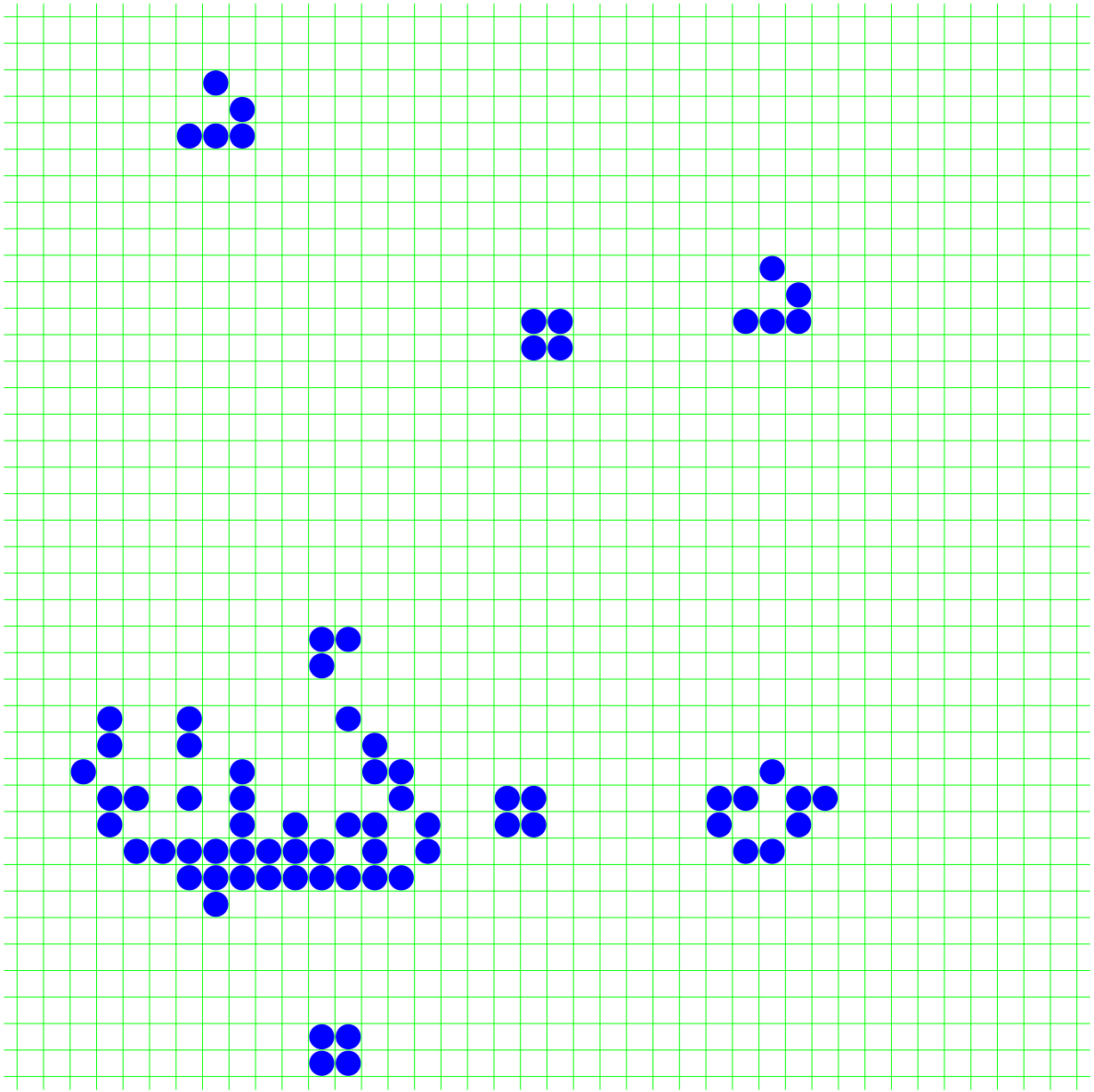

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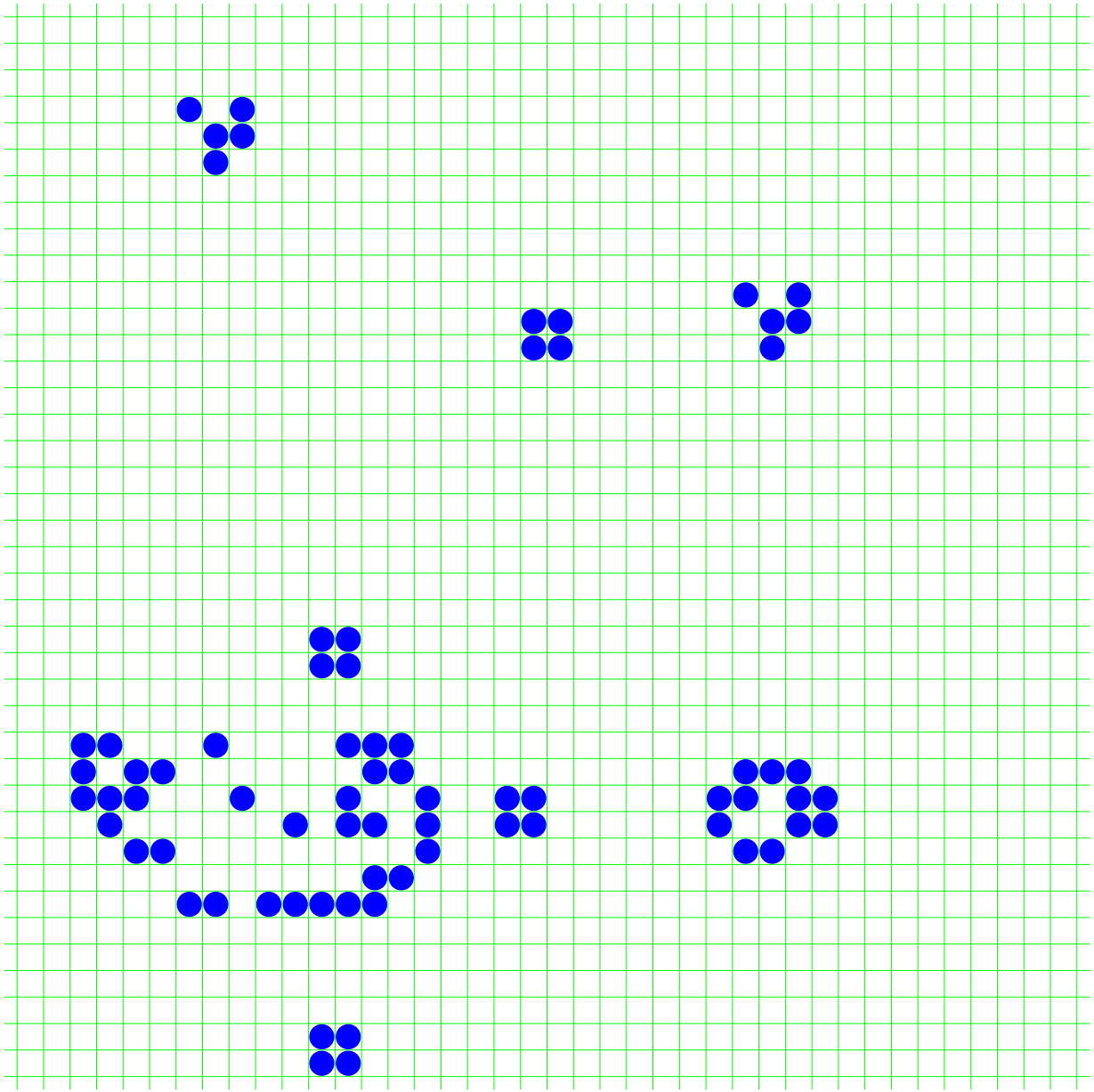

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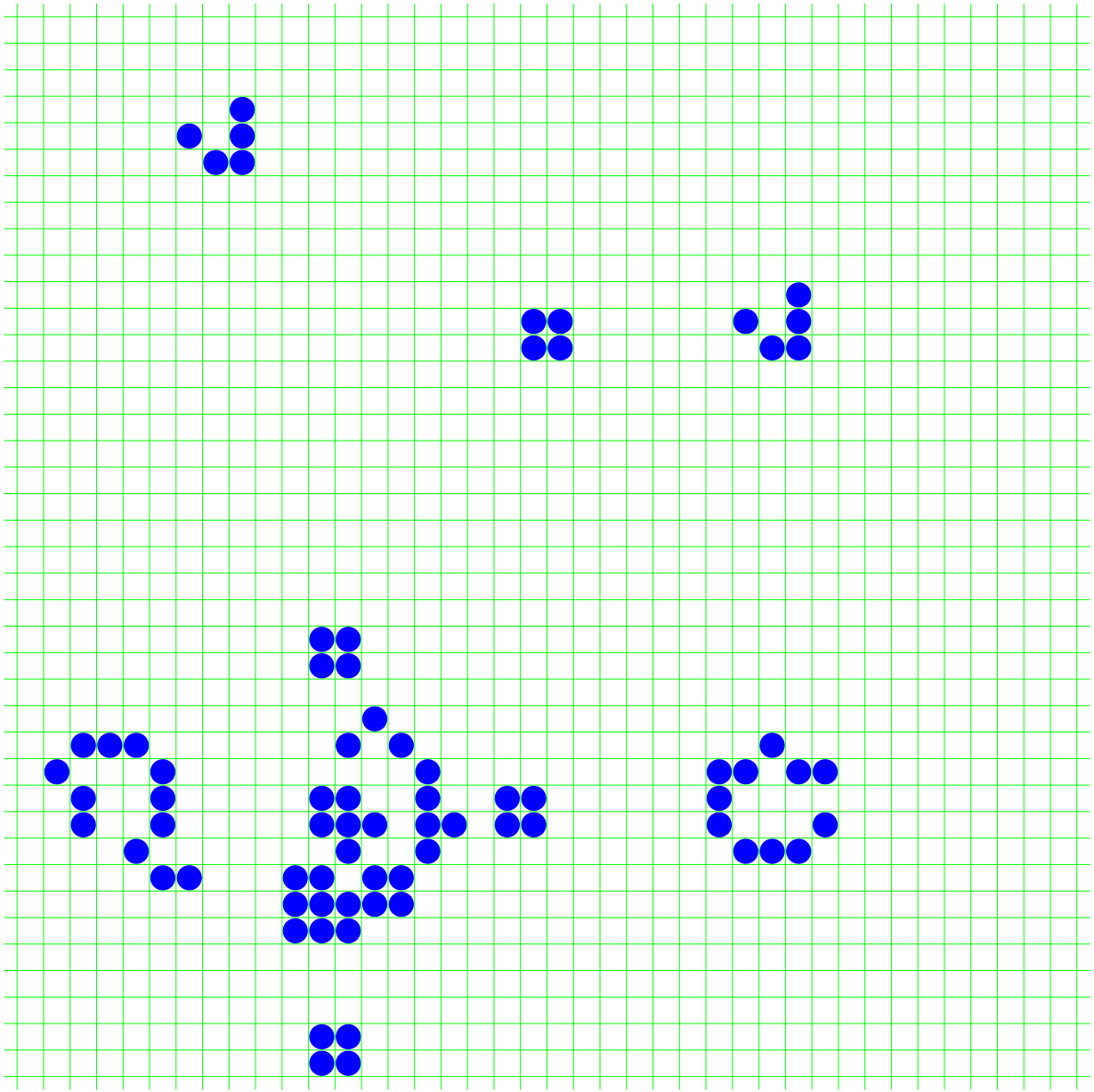

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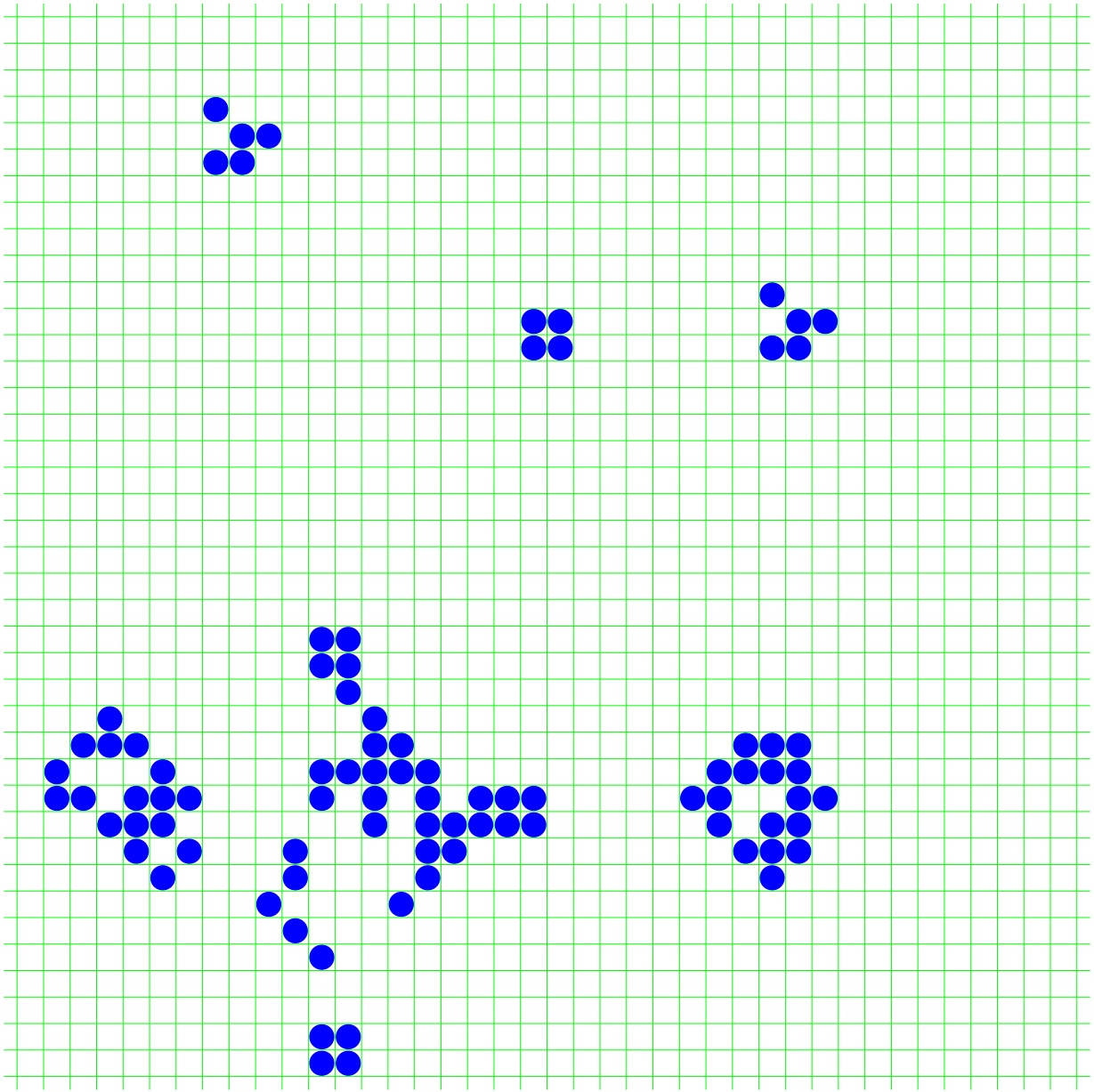

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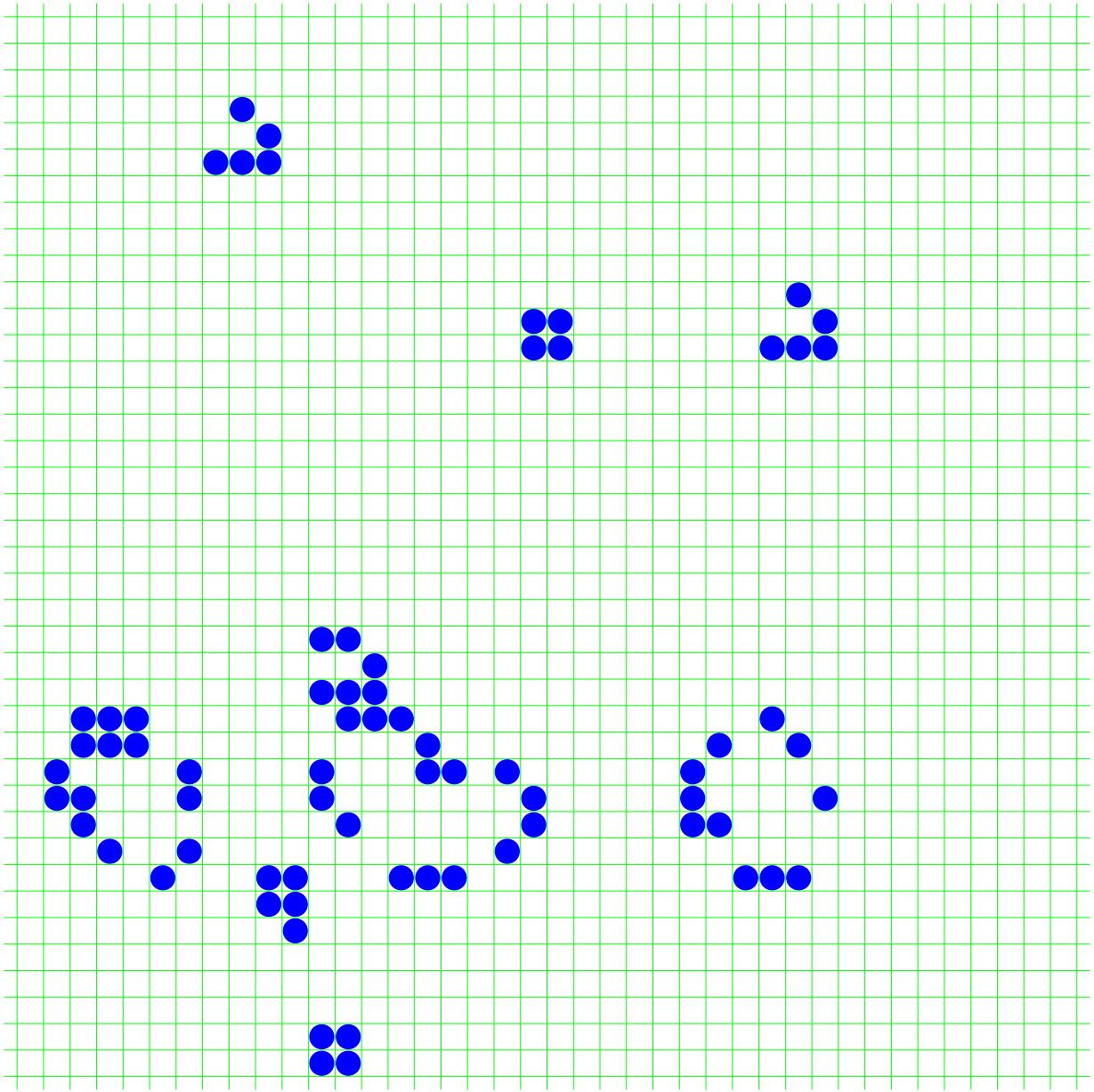

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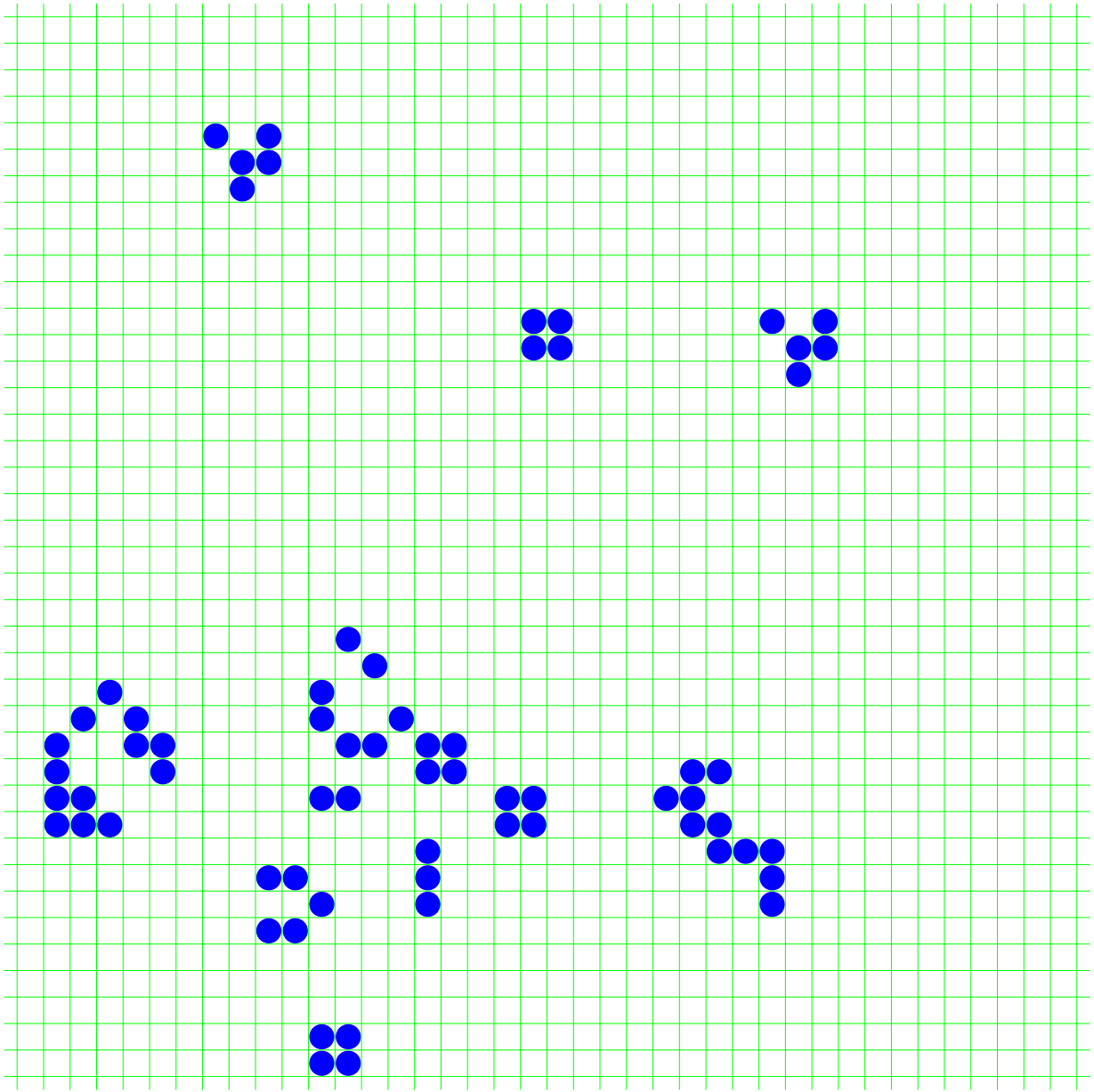

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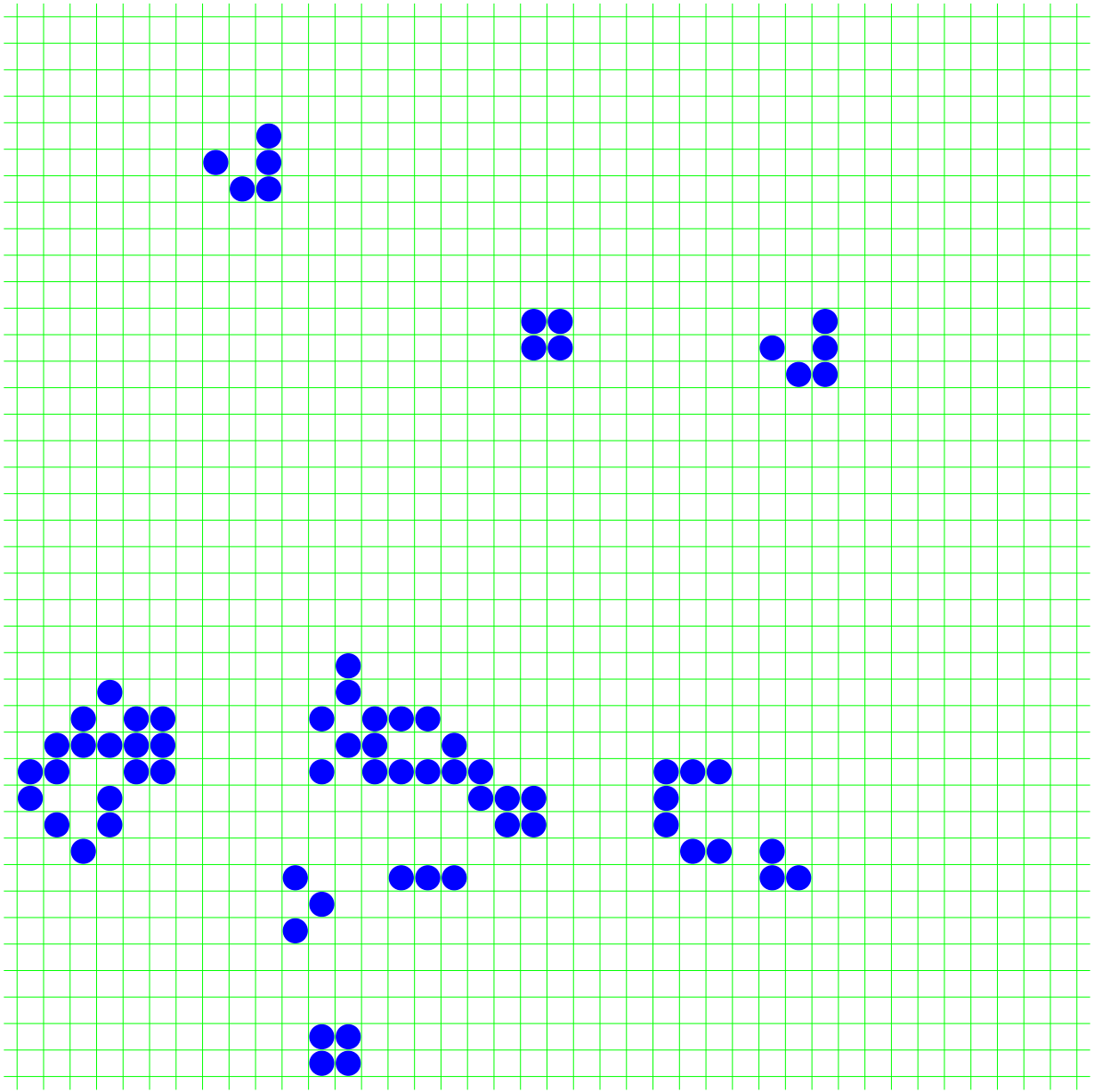

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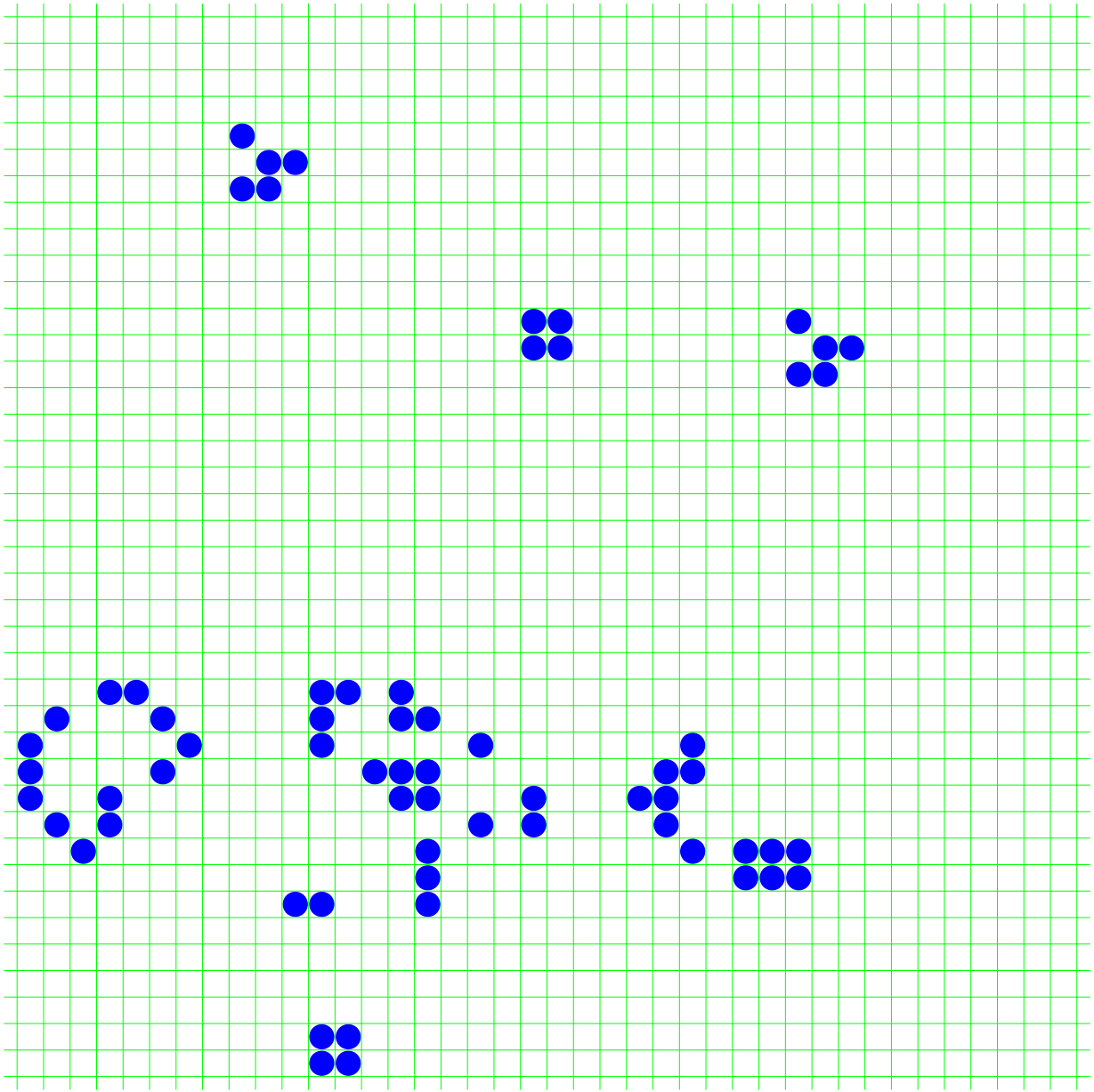

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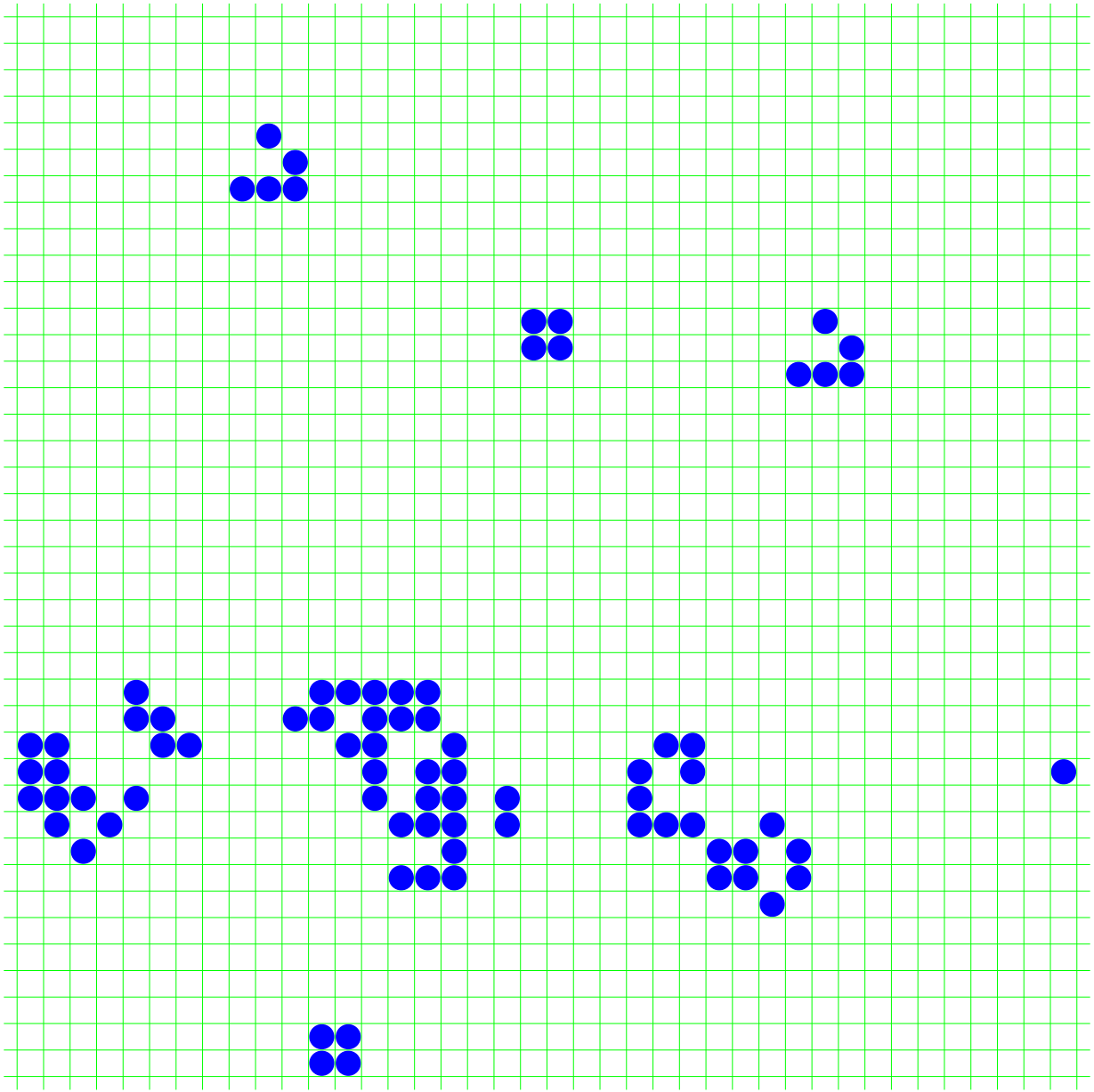

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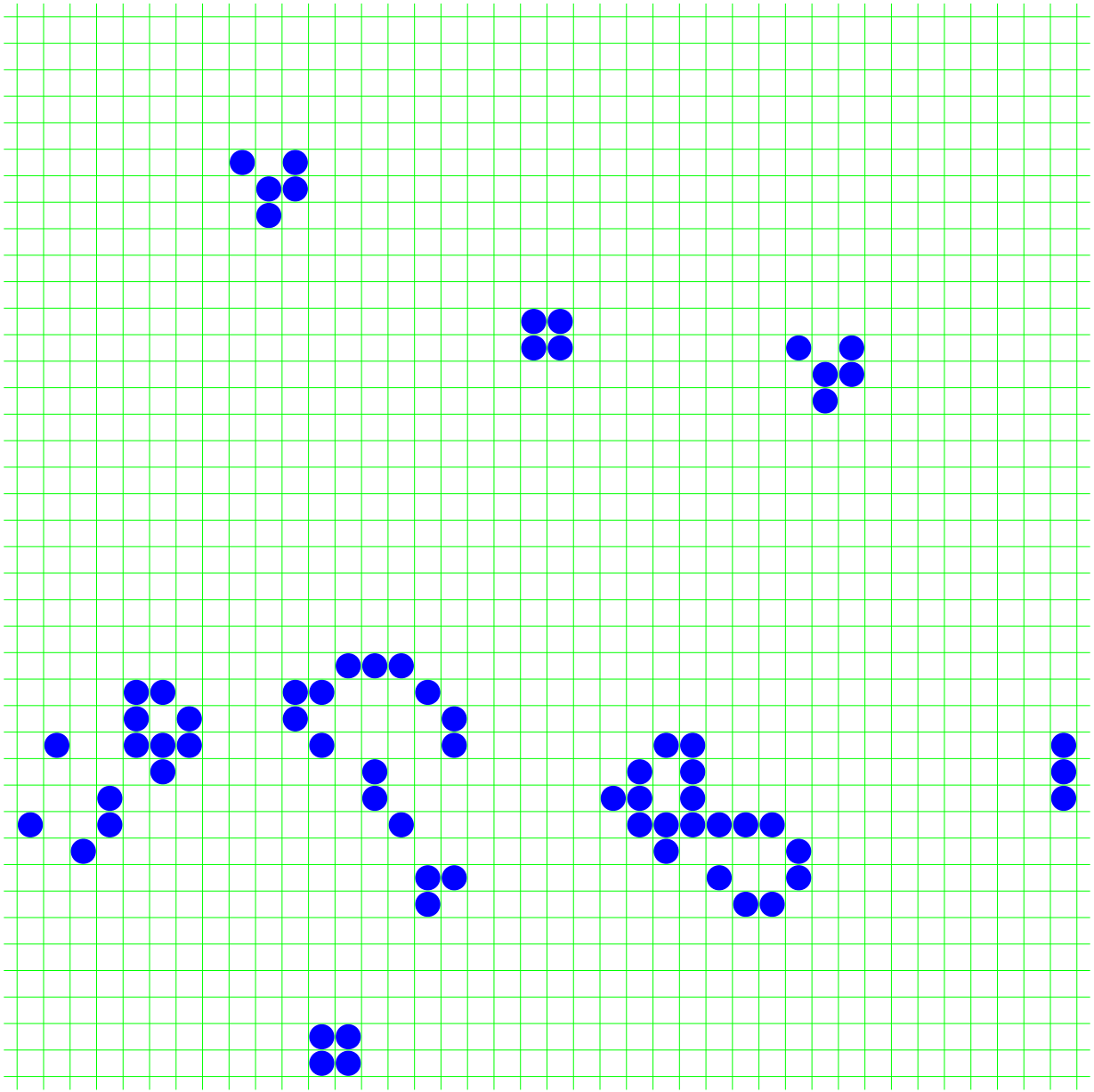

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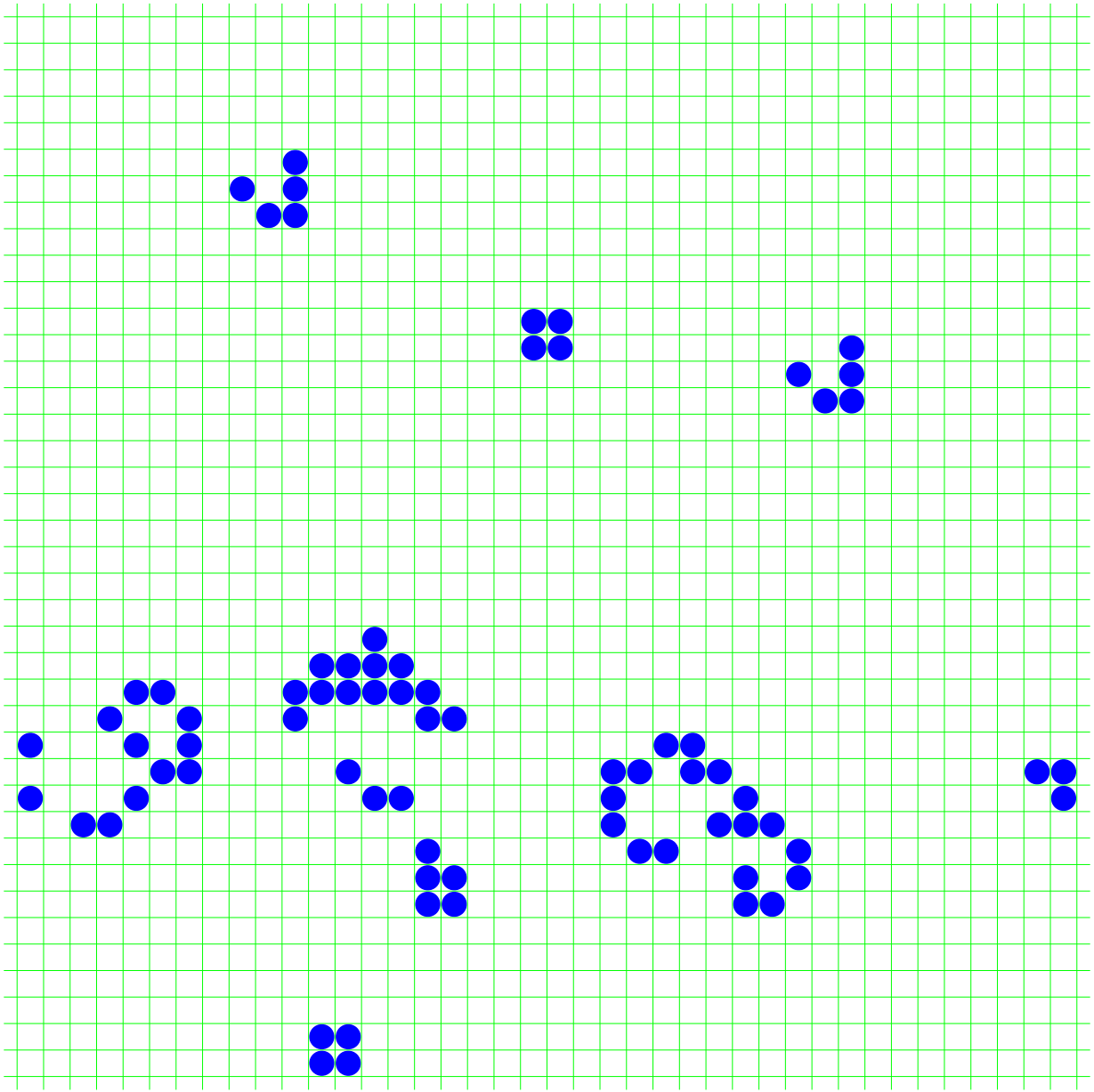

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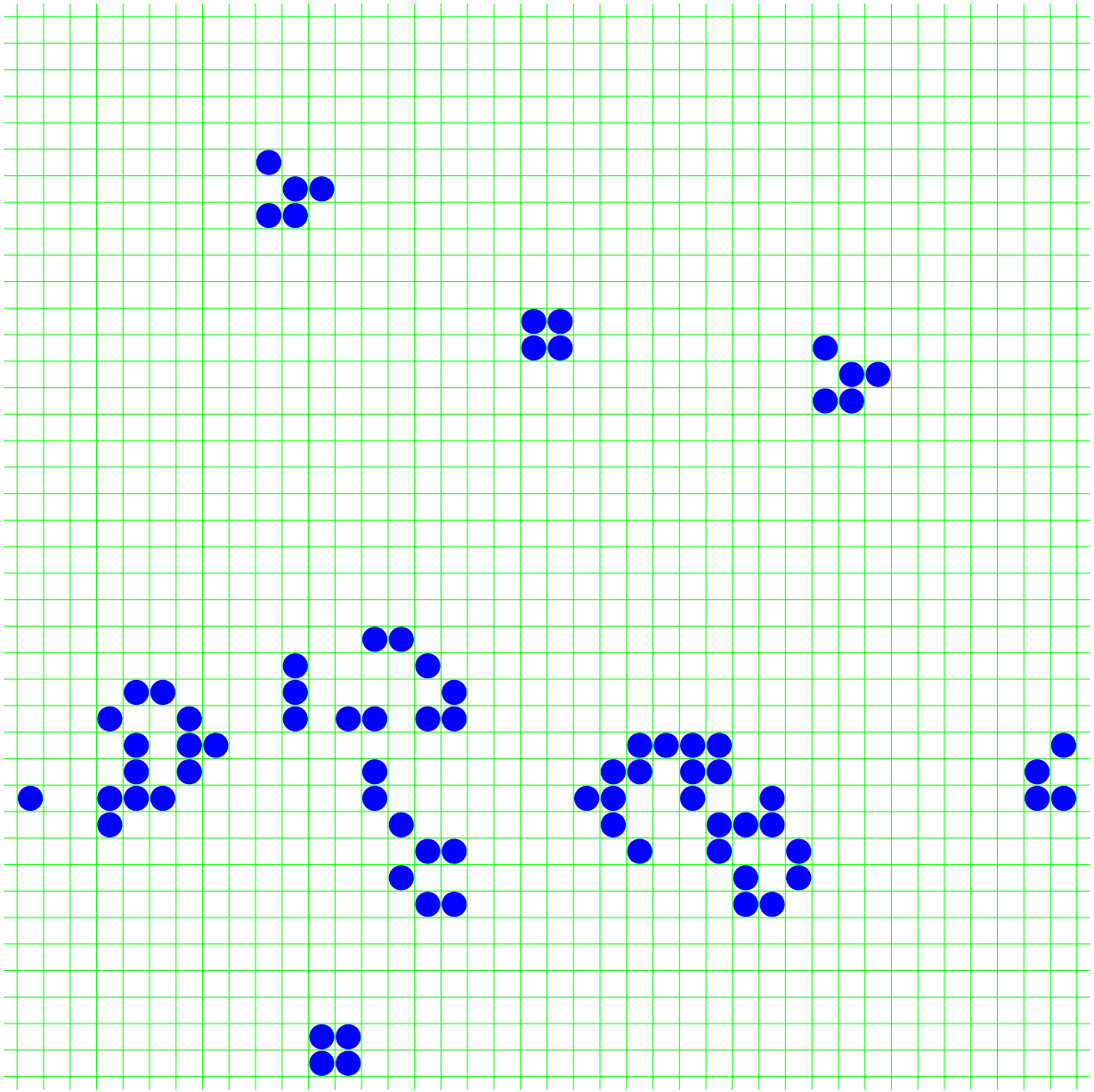

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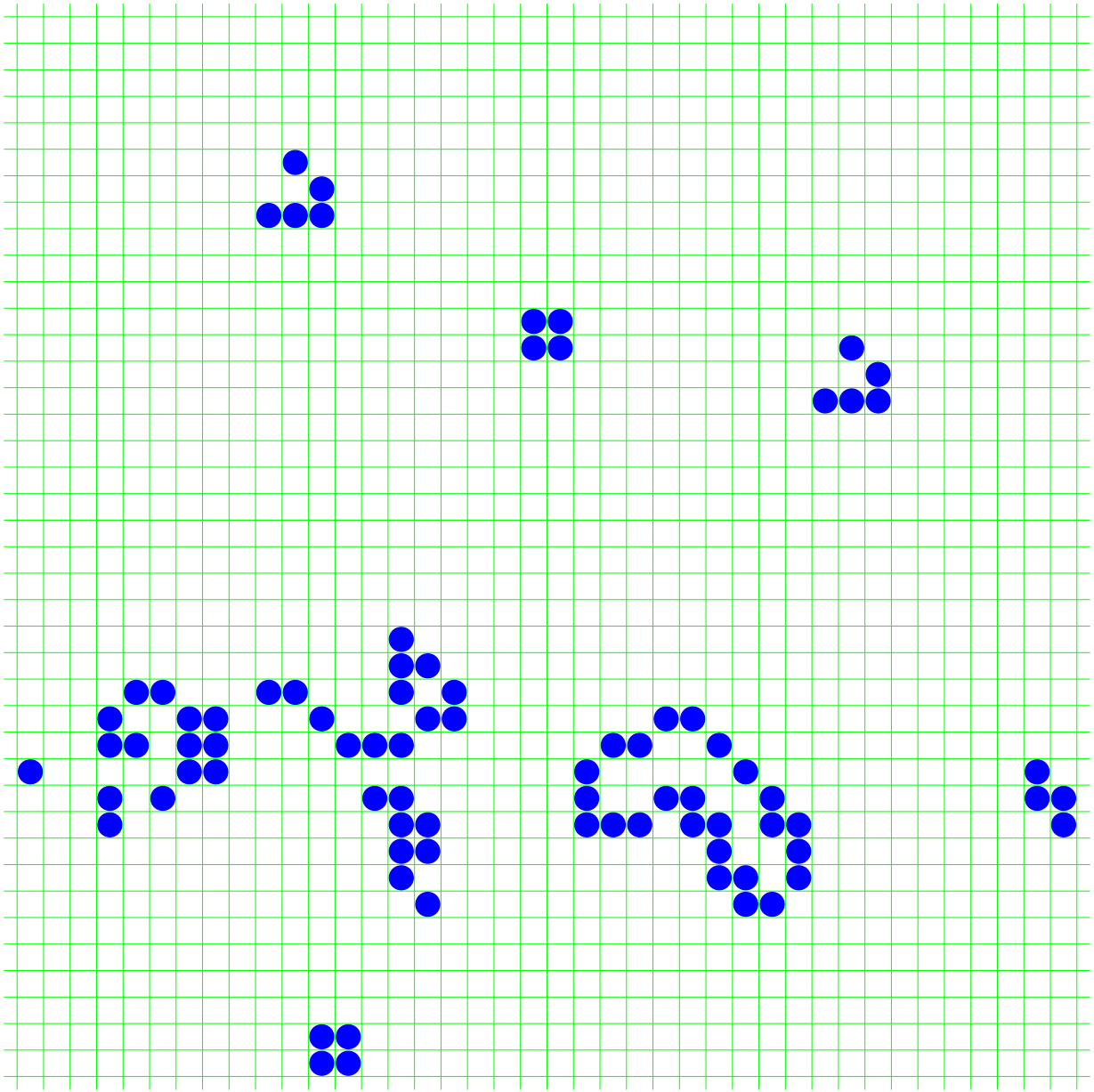

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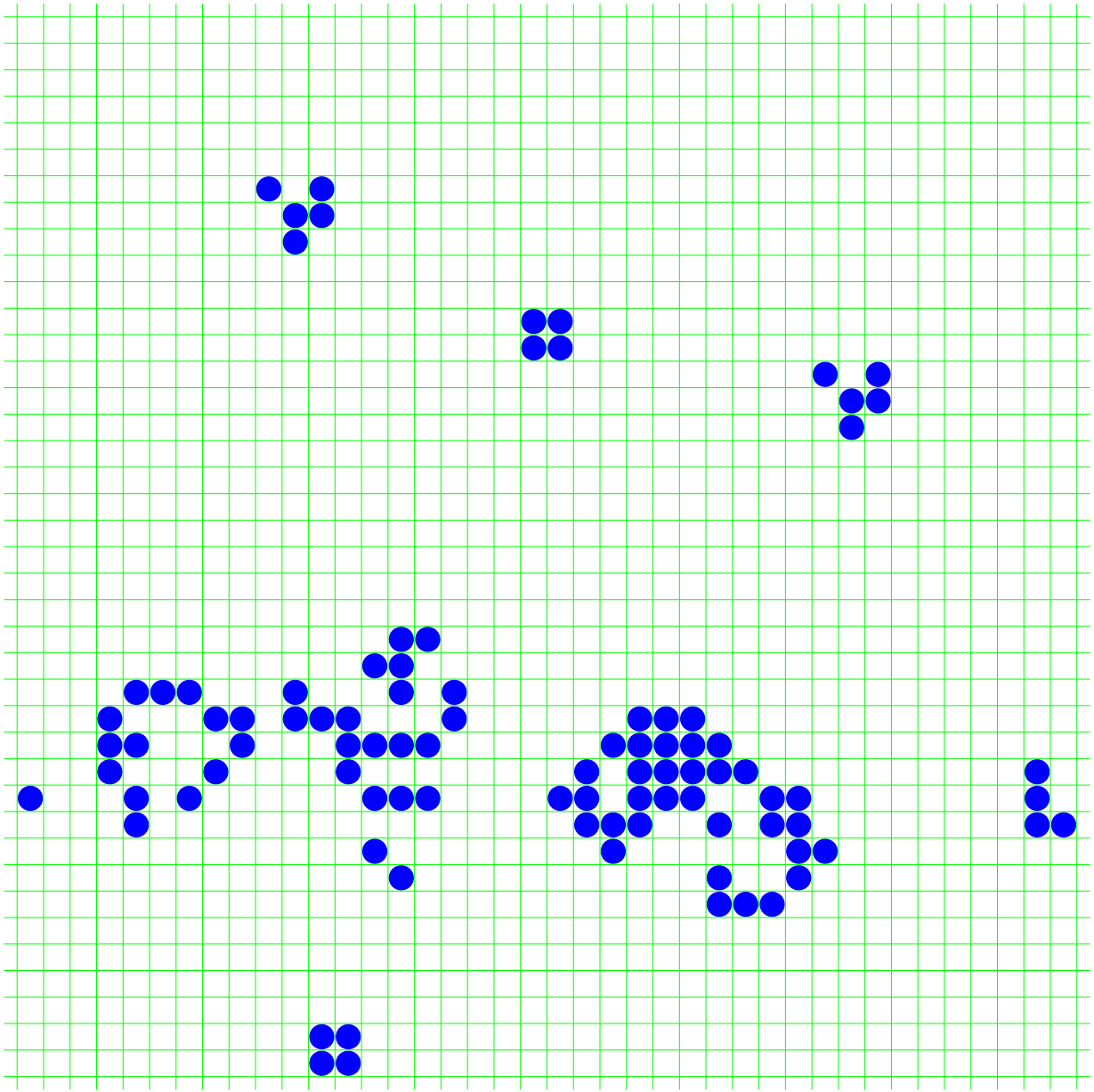

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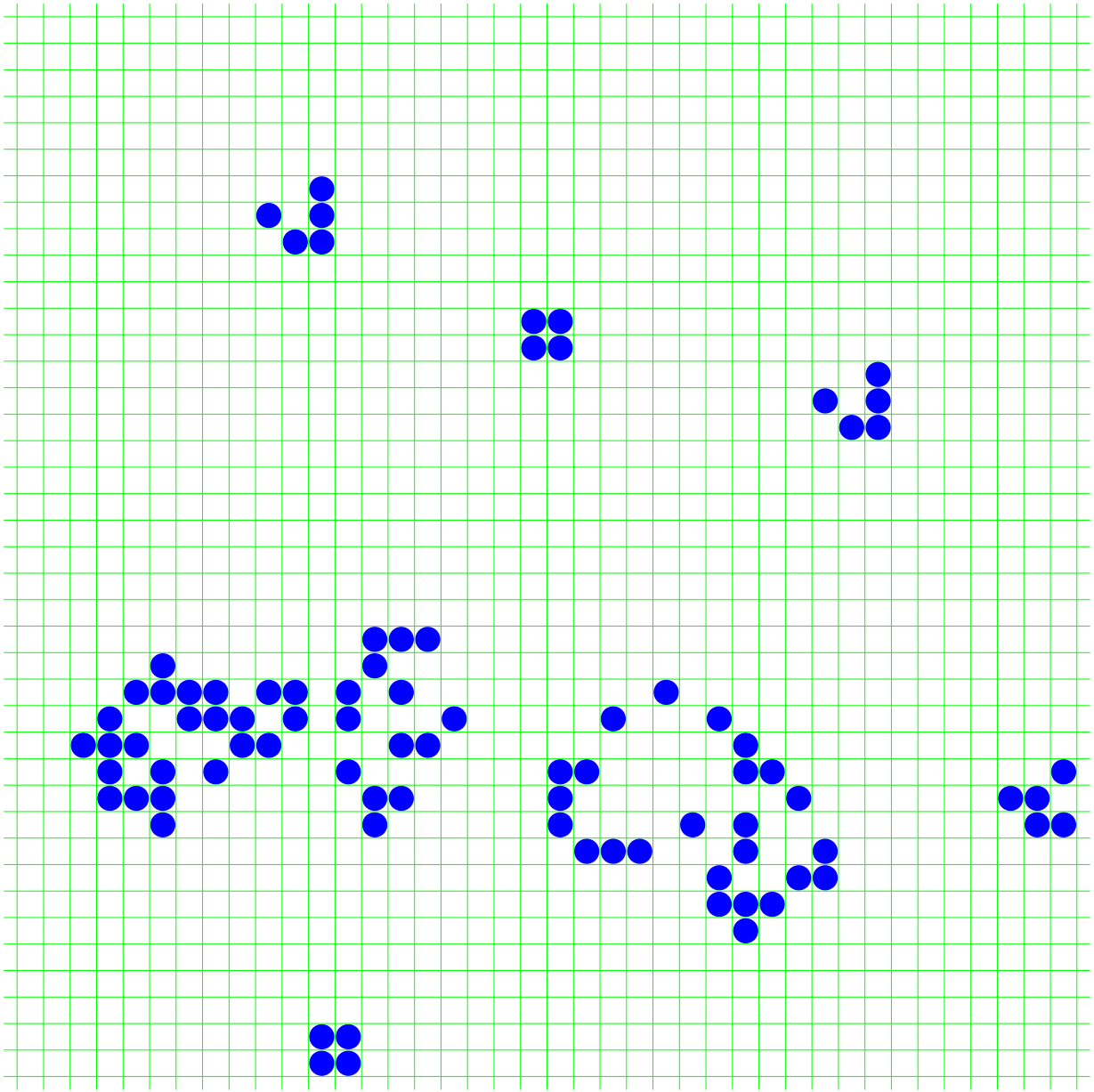

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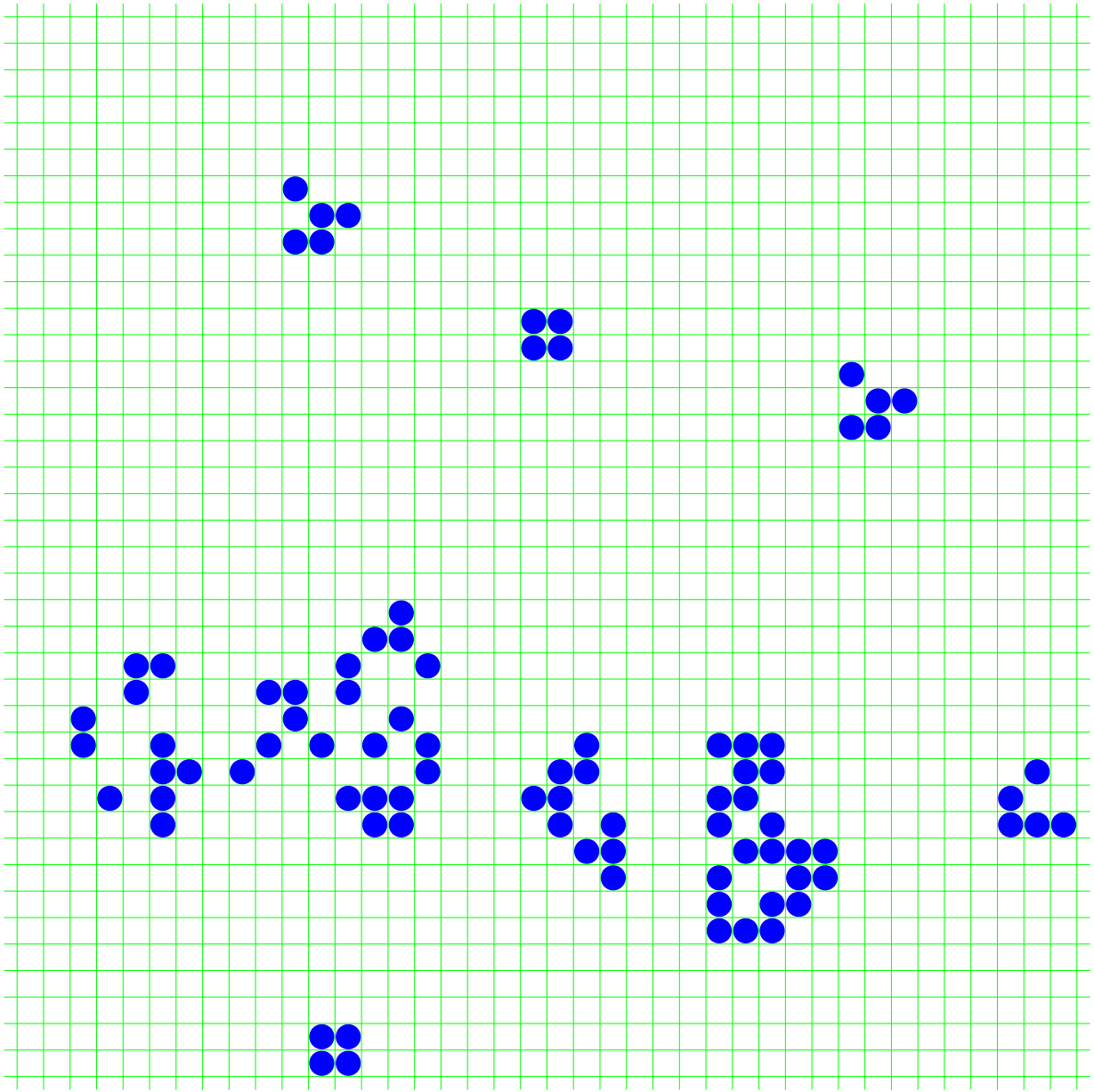

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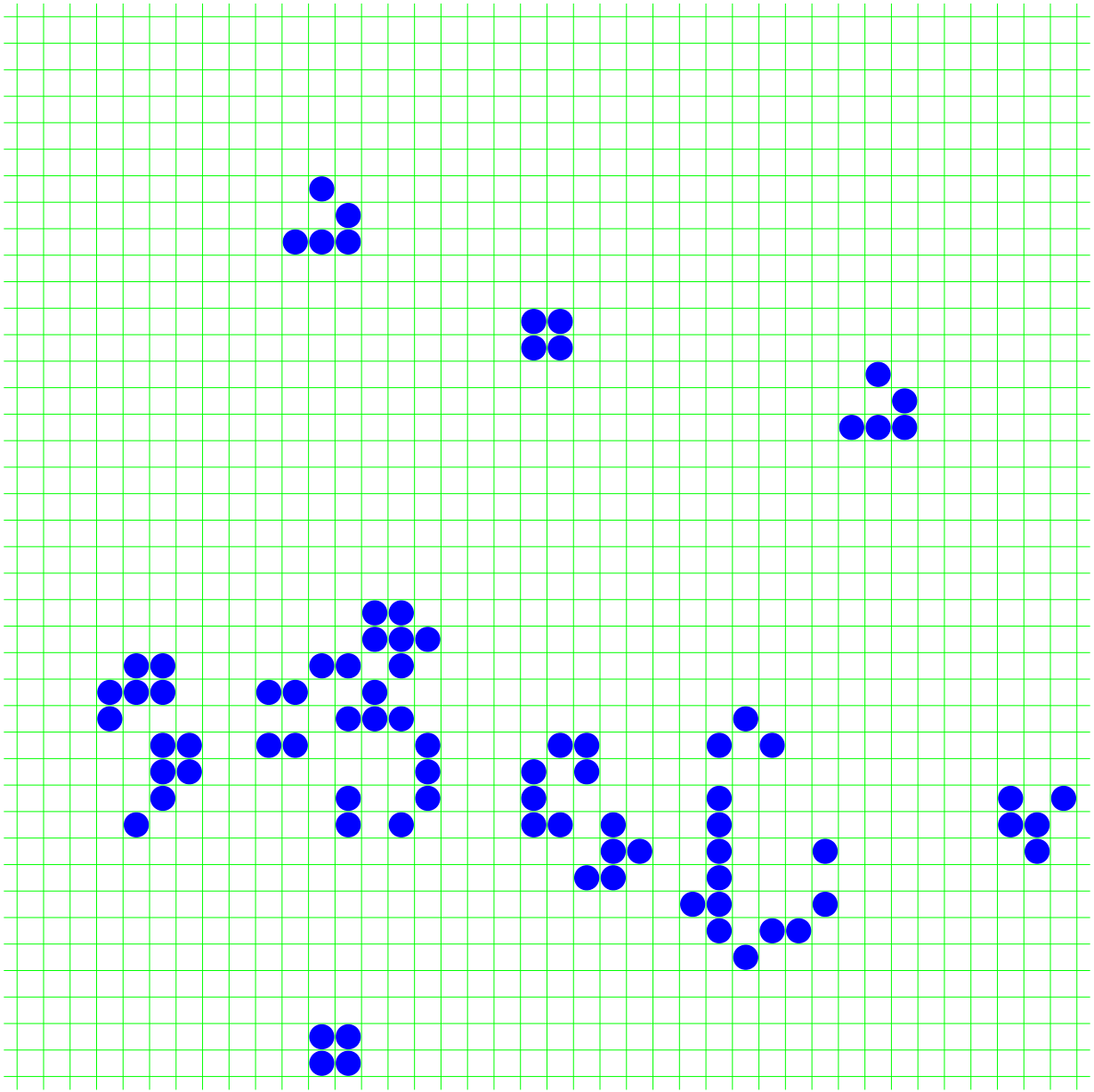

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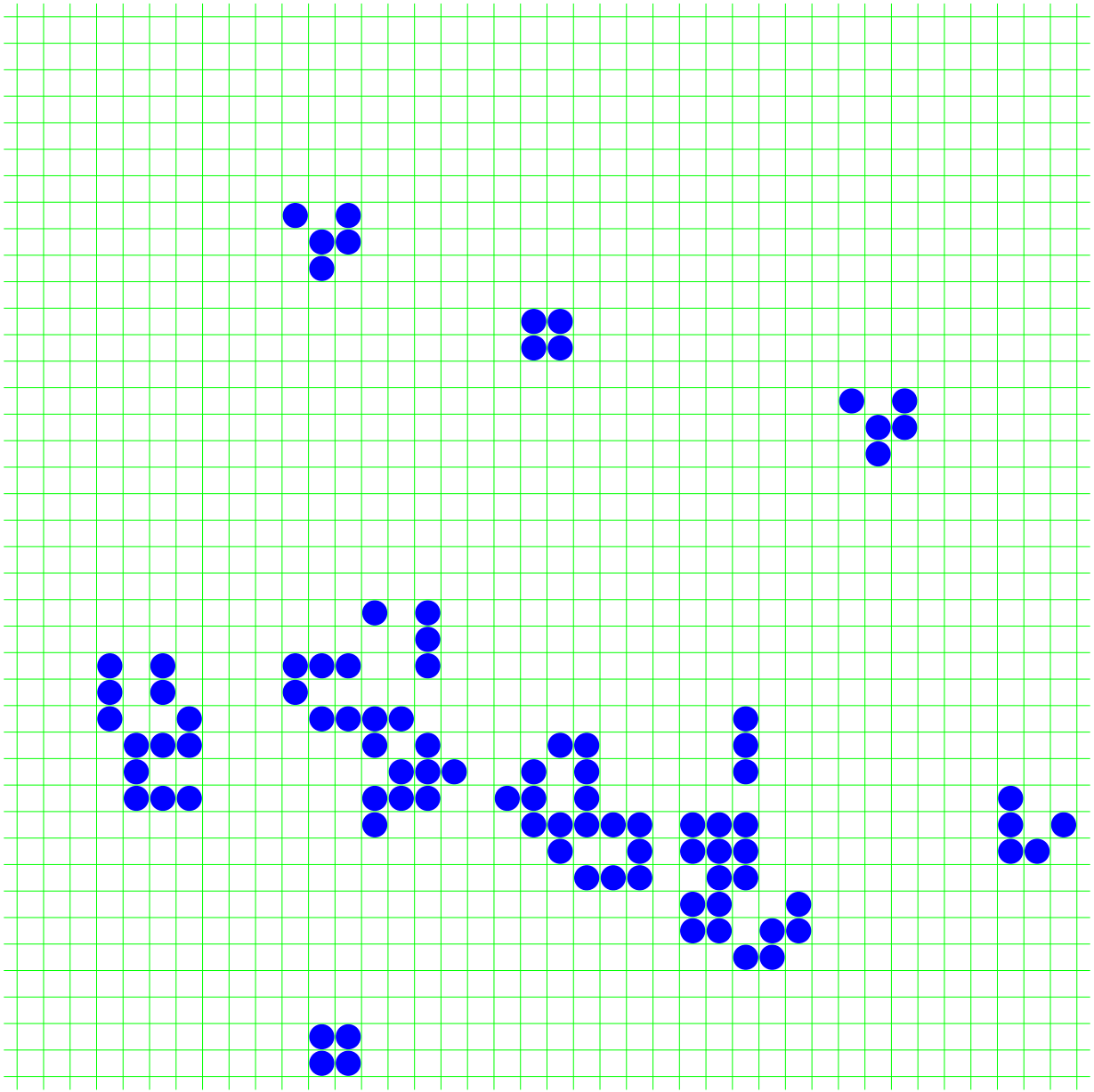

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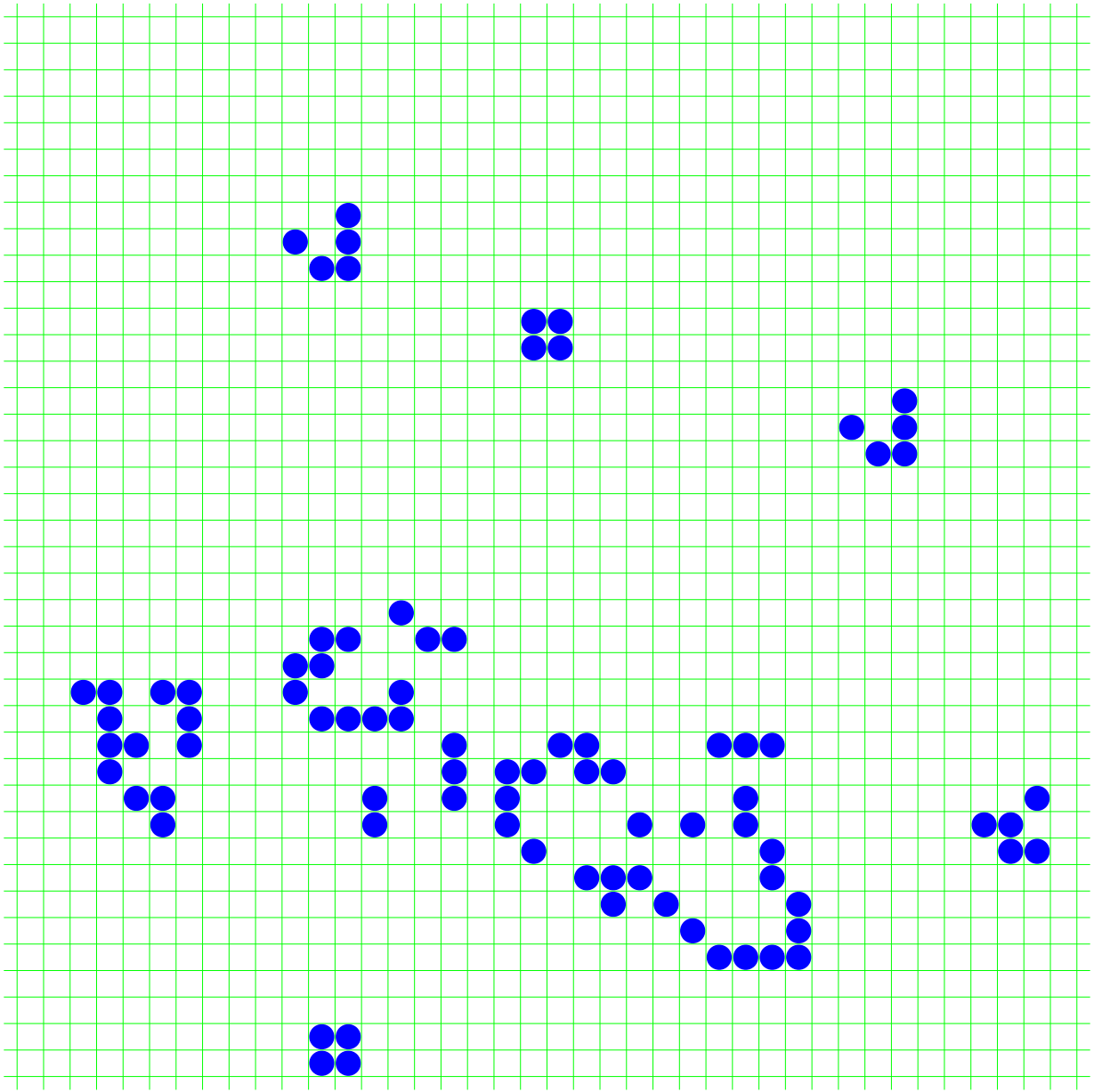

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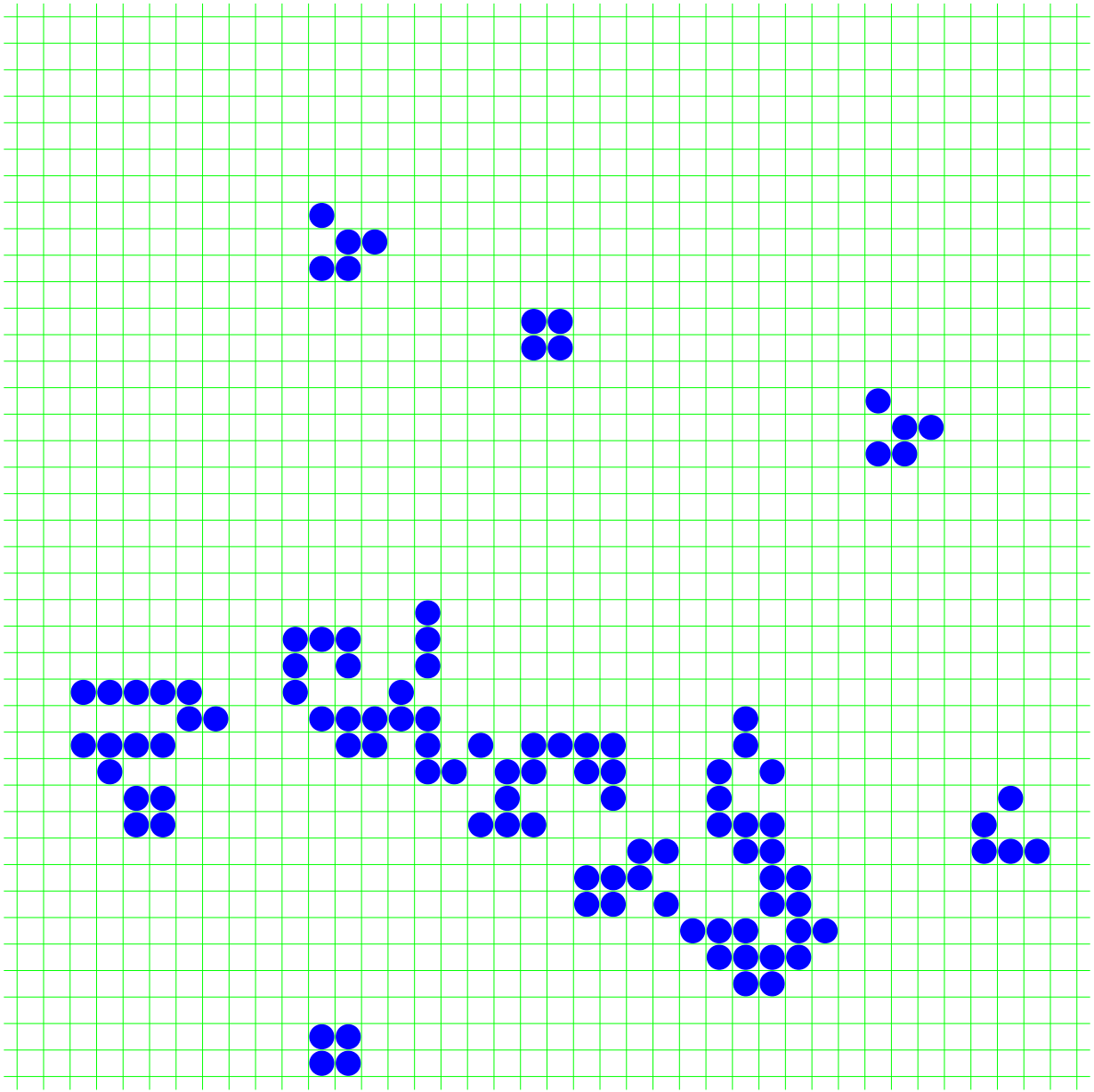

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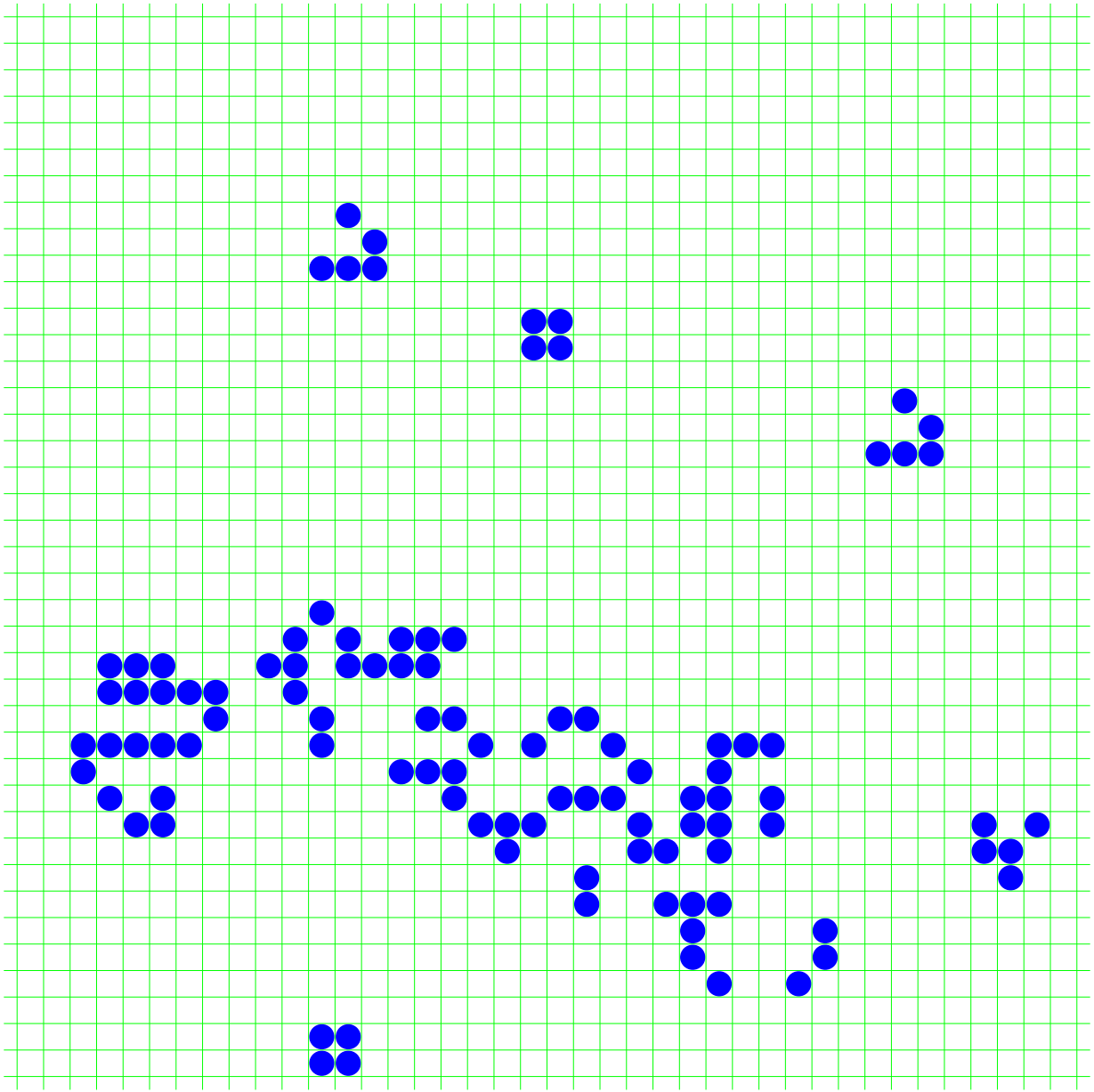

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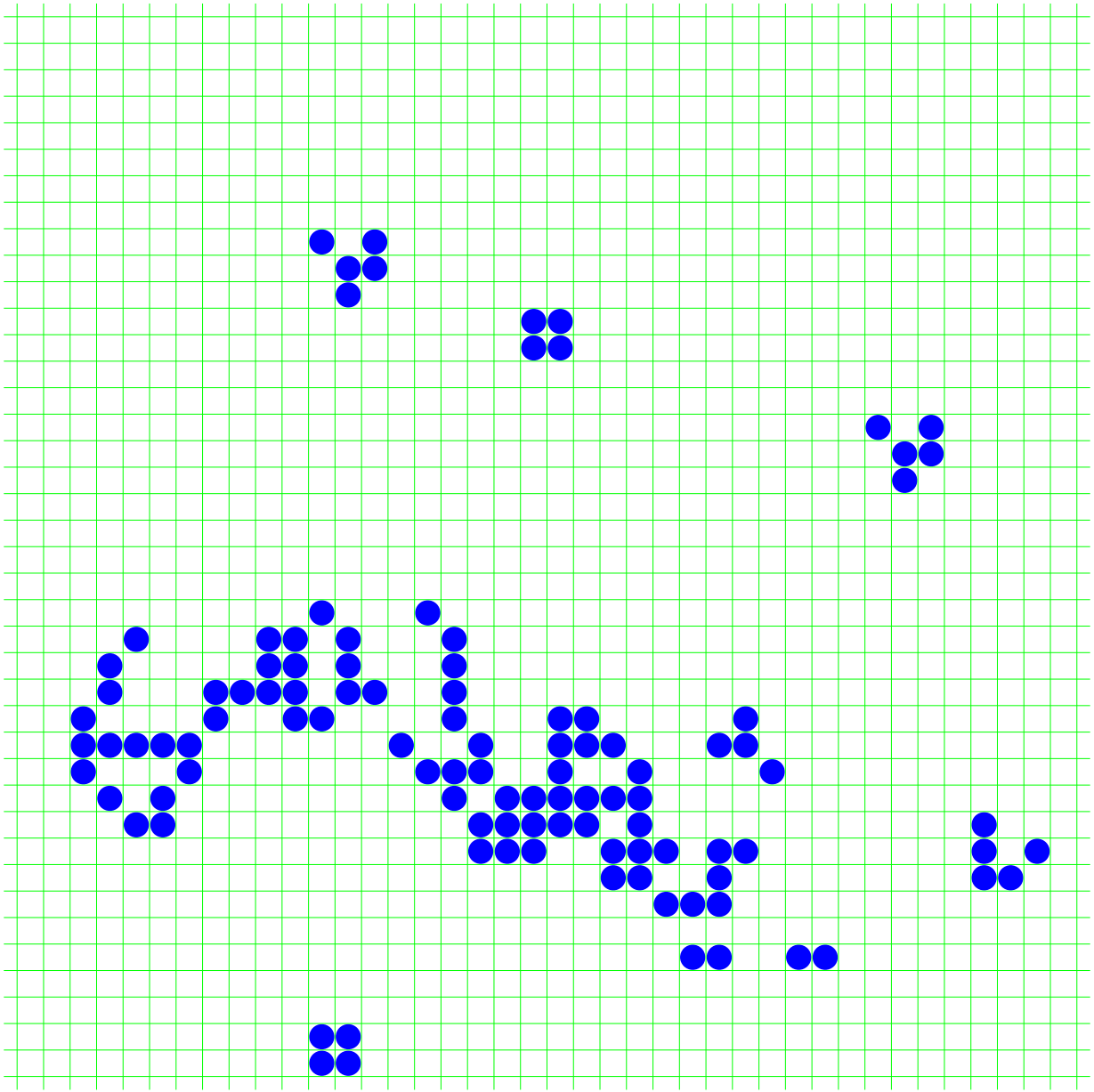

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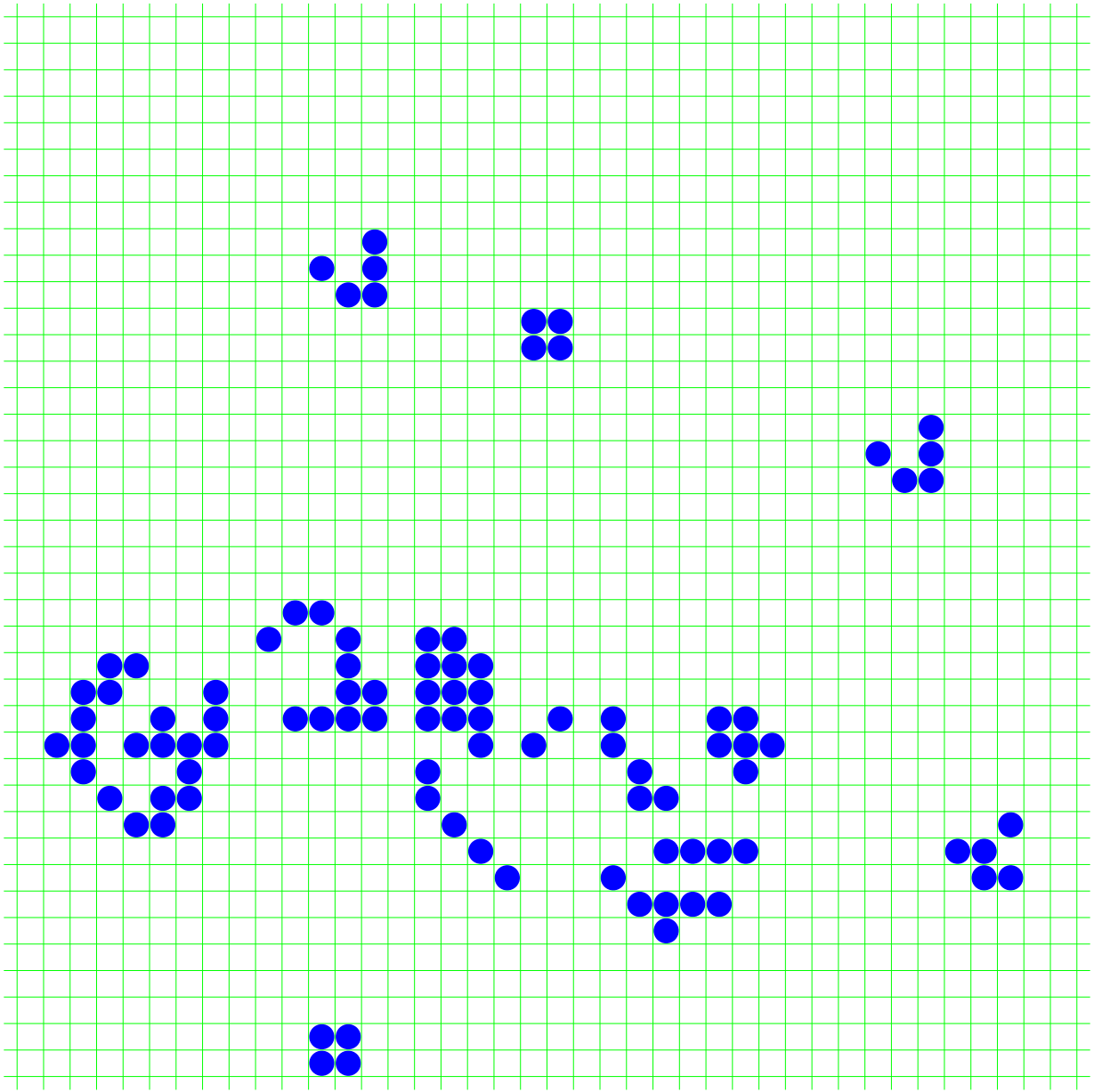

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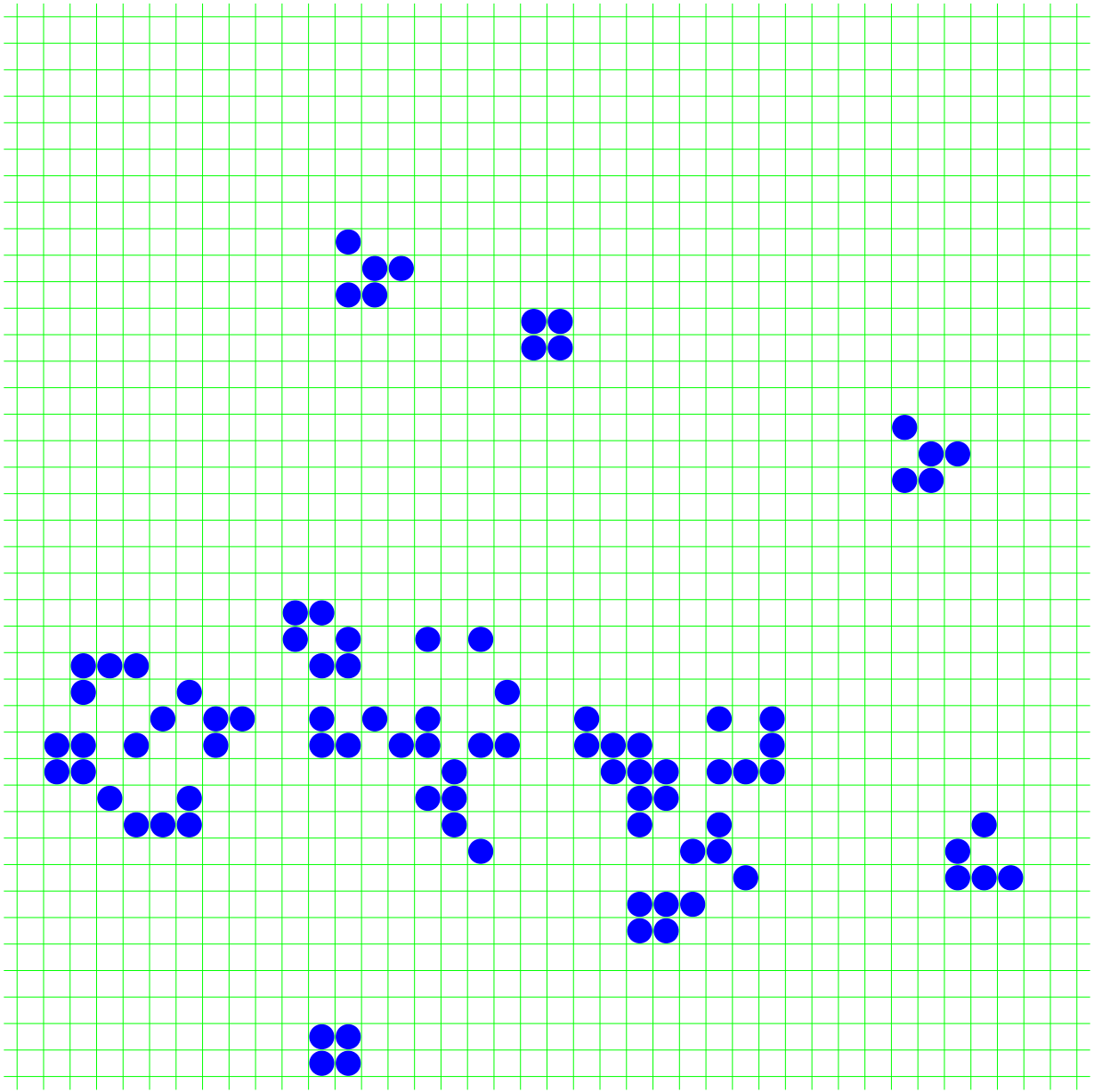

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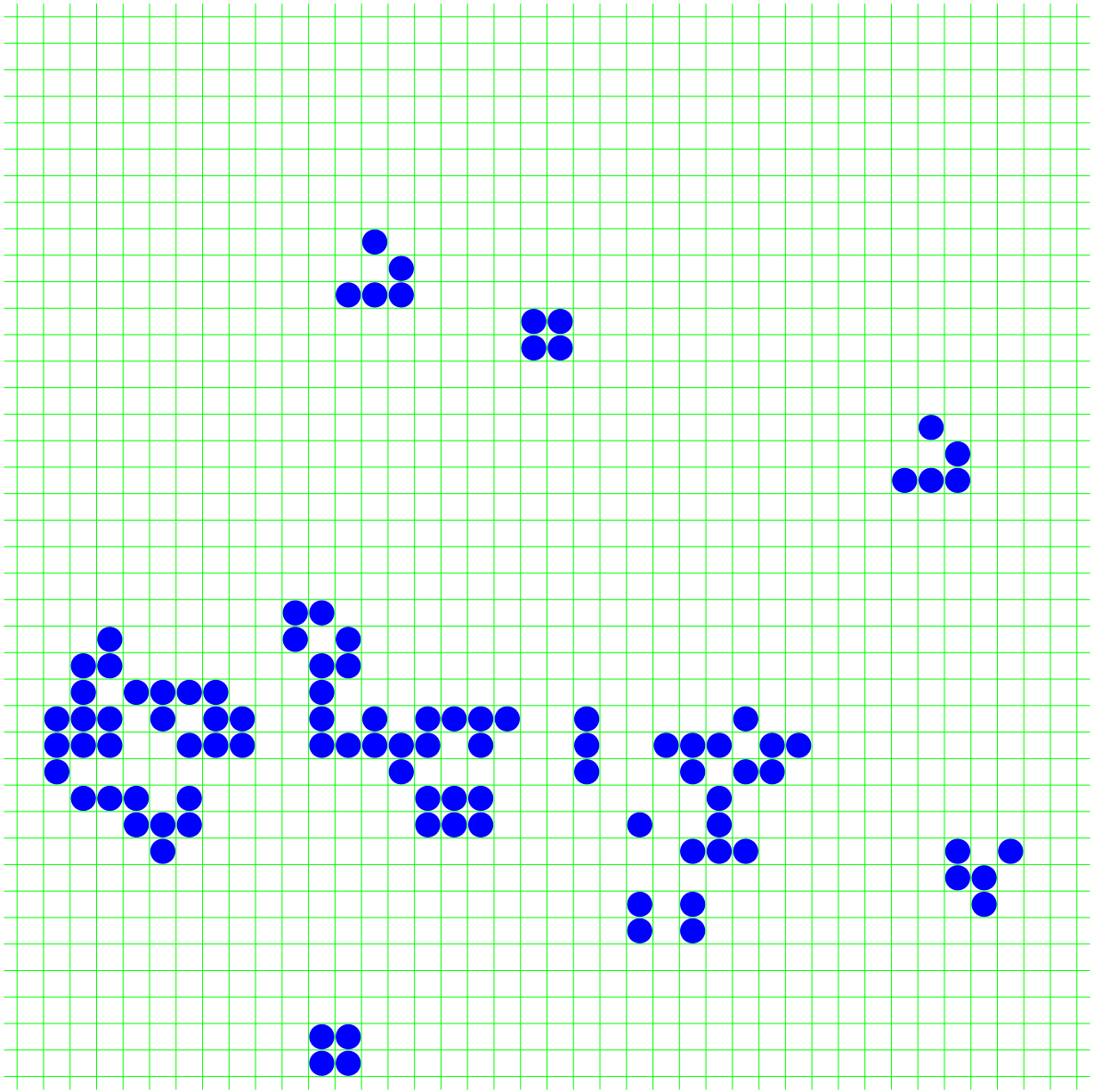
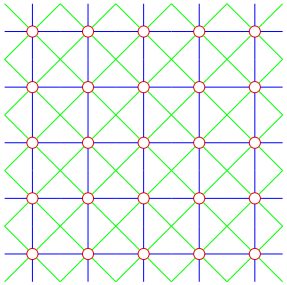


Symmetries of Toric $N \times N$ Square Lattices $X_{N\times N}$

$X_{N\times N} =$  has the same group $G_{N\times N}$ in both 4-valent von Neumann and 8-valent Moore cases

Principal case $N = 3, 5, 6, \ldots, \infty$ $\quad |G_{N\times N}| = 8N^2$ $\quad \mathbf{T}^2$ is normal

$G_{N\times N} = \mathbf{T}^2 \rtimes \mathrm{D}_8$ — semidirect product of $\mathbf{T}^2$ and D_8
$\mathbf{T}^2 = \mathbb{Z}_N \times \mathbb{Z}_N$ — translation group ($\mathbb{Z}_\infty \equiv \mathbb{Z}$)
$\mathrm{D}_8 = \mathbb{Z}_4 \rtimes \mathbb{Z}_2$ — dihedral group ($\mathbb{Z}_4$ – 90^0 rotations, $\mathbb{Z}_2$ – reflections)
Resembles Euclidean group $\mathbf{E}_2 = \left(\mathbf{T}^2 = \mathbb{R} \times \mathbb{R}\right) \rtimes \mathbf{O}(2)$

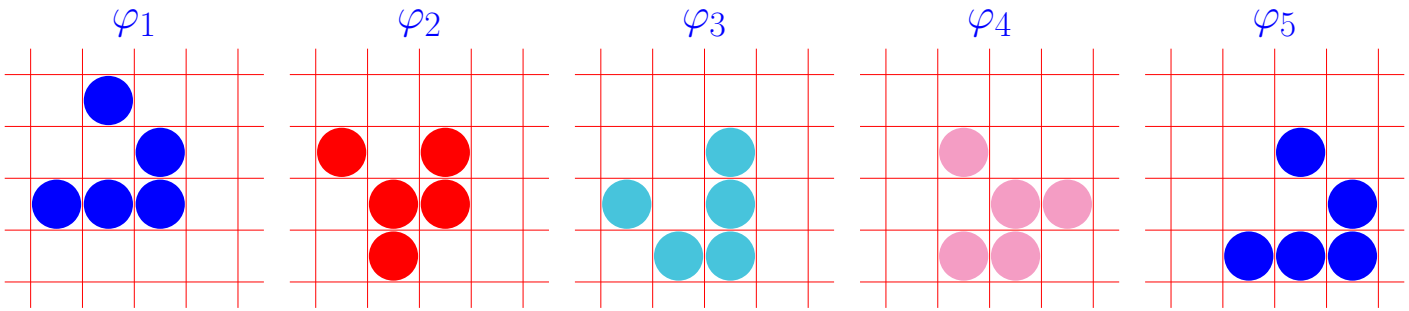
Exception: $N = 4$ $\quad |G_{N\times N}| = 3 \times 8N^2$ $\quad \mathbf{T}^2$ is not normal

$$G_{4\times 4} = \overbrace{((((\mathbb{Z}_2 \times \mathrm{D}_8) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_3) \rtimes \mathbb{Z}_2)}^{\text{normal closure of } \mathbf{T}^2} \rtimes \mathbb{Z}_2 \quad \text{(by GAP algorithm)}$$

Group Interpretation of "Glider"

Evolution operator = group action: $\varphi_{t_b}(x) = A_{t_a t_b}\left(\varphi_{t_a}(x)\right) = \varphi_{t_a}\left(g^{-1}_{t_a t_b} x\right)$

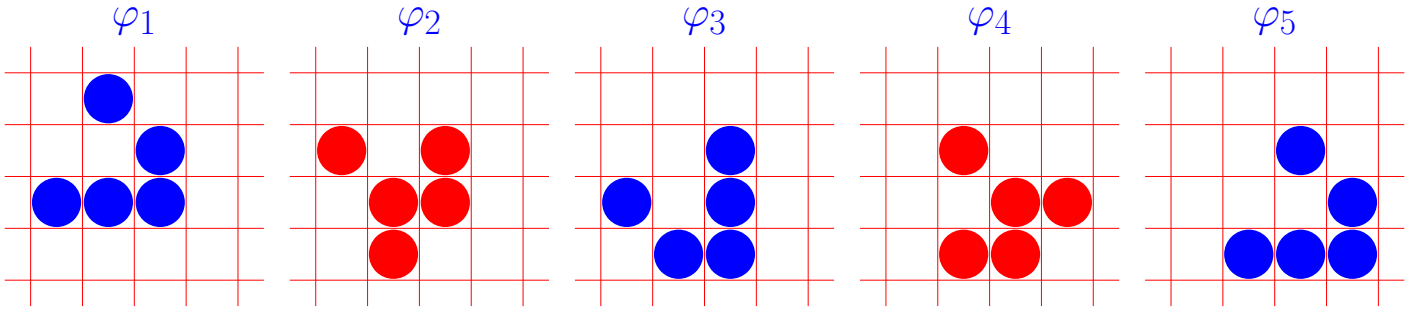
One step diagonal shift $\quad g_{15} \in \mathbf{T}^2$



"Glider" over translation group $\mathbf{T}^2$ is cycle in 4 orbits

One step downward shift $\rightarrow$ 90° clockwise rotation $\rightarrow$ reflection in respect to vertical

$$g_{13} = g_{24} \in \mathbf{T}^2 \rtimes \mathrm{D}_8$$



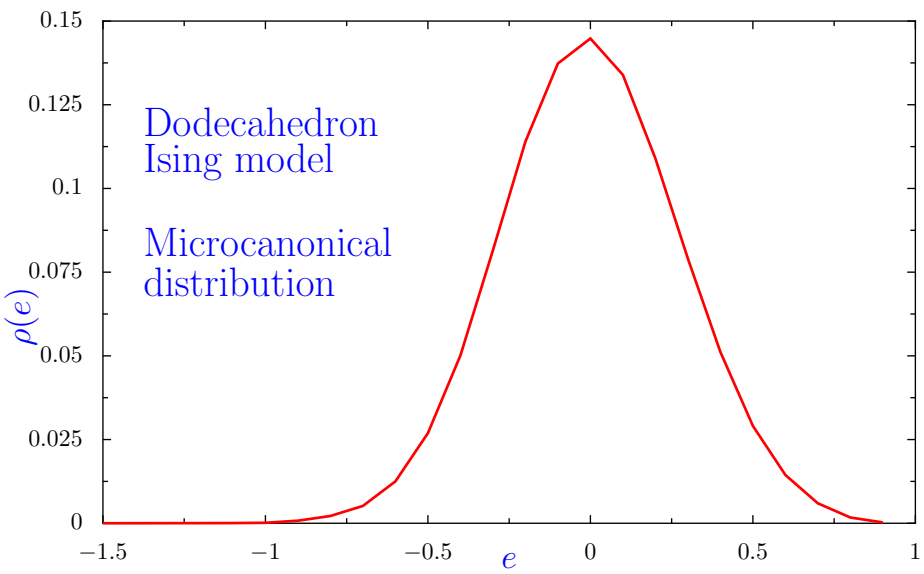
"Glider" over maximal symmetry group $\mathbf{T}^2 \rtimes \mathrm{D}_8$ is cycle in 2 orbits

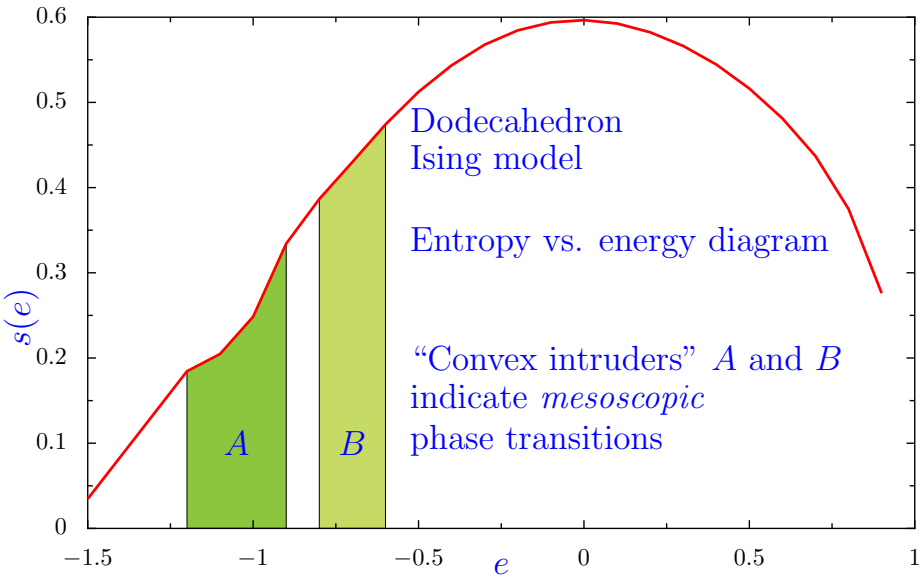
Mesoscopic Lattice Models

Discrete symmetry analysis simplifies manipulations with microcanonical ensembles and search of phase transitions.

This allows to reveal subtle details in behavior of mesoscopic models:

in the figure in addition to distinct "convex intruder" — criterion of phase transition adopted in mesoscopy — denoted A computation detects subtle "intruder" B.





Gauge Principle

Birth of idea: Hermann Weyl, 1918

Start of modern development: Chen Ning Yang & Robert Mills, 1954

All fundamental physical theories are gauge theories

Theory	Gauge Group
Gravity	Poincaré group $\mathbb{R}^4 \rtimes \mathrm{O}(1,3)$
Electrodynamics	$\mathrm{U}(1)$
Electroweak Theory	$\mathrm{U}(1) \times \mathrm{SU}(2)$
Quantum Chromodynamics	$\mathrm{SU}(3)$
Standard Model	$\mathrm{U}(1) \times \mathrm{SU}(2) \times \mathrm{SU}(3)$

Constructive Versions of Gauge Theories

In 1974 K.G. Wilson introduced lattice gauge theory

as practical computational approach to problems of strong interactions for which standard perturbative methods are inapplicable.

Later mathematical development established relations between lattice gauge theories and: topological quantum field theory (TQFT), invariants of 3- and 4-manifolds, monoidal categories, Hopf algebras and quantum groups, quantum gravity etc.

Above mentioned lattice theories are not entirely discrete

They involve continuous ingredients: gauge groups are Lie groups, Lagrangians and observables are real (or complex) functions.

Here we will try to formulate discrete gauge models and their quantization in purely constructive terms.

Gauge Principle at Set-theoretic Level. I

Consideration without Fiber Bundles and Differentiable Structures

- Space X
- Local states Σ
- States Σ^X of the whole system — Σ-valued functions on X
- Group $W \leq \mathrm{Sym}\left(\Sigma^X\right)$ acting transitively on Σ^X
  — symmetries of system
- Identification of data describing dynamical system with states from Σ^X makes sense only *modulo* symmetries from W
- Having no *a priori* connection between data from Σ^X at different points x and y in time and space we impose this connection (or parallel transport) explicitly as W-valued functions on edges of *abstract* graph:

$$P(x,y) \in W, \ \varsigma(y) = \sigma(x)P(x,y)$$

Obviously $P(y,x) = P(x,y)^{-1}$

Gauge Principle at Set-theoretic Level. II

- Connection $P(x, y)$ is called trivial if it can be expressed in terms of a function on vertices of graph:
$$P(x, y) = r(x)^{-1} r(y), \; r(x), r(y) \in W$$
- Invariance wrt gauge symmetries depending on time or space $u(x), u(y) \in W$ leads to transformation rule for connection
$$P(x, y) \to u(x)^{-1} P(x, y) u(y)$$
- Curvature of connection $P(x, y)$ is defined as the conjugacy class of holonomy along a cycle of graph:
$$P(x_1, x_2, \ldots, x_k) = P(x_1, x_2) P(x_2, x_3) \cdots P(x_k, x_1)$$

  Conjugacy means $P'(x_1, \ldots, x_k) \sim u^{-1} P(x_1, \ldots, x_k) u$ for any $u \in W$
  Curvature of trivial connection is obviously: $\widetilde{P}(x_1, \ldots, x_k) \equiv 1$
- Gauge principle provides no idea about dynamics of connection (gauge field) itself — suitable relations should be added

Electrodynamics. Abelian prototype of all gauge theories. I

- X is 4-dimensional Minkowski space with points $x = (x^\mu)$
- States Ψ^X form Hilbert space of complex fields $\psi(x)$
- Gauge group $W = U(1)^X$ consists of elements $e^{-i\alpha(x)}$
- Parallel transport for two closely situated space-time points

$$P(x, x + \Delta x) = e^{-i\rho(x, x+\Delta x)}$$

- Specializing general rule $P(x, y) \to u(x)^{-1} P(x, y) u(y)$:

$$P'(x, x + \Delta x) = e^{i\alpha(x)} P(x, x + \Delta x) e^{-i\alpha(x+\Delta x)},$$

substituting approximations

$$\begin{aligned} P(x, x + \Delta x) &= e^{-i\rho(x, x+\Delta x)} \approx 1 - iA(x)\Delta x \\ P'(x, x + \Delta x) &= e^{-i\rho'(x, x+\Delta x)} \approx 1 - iA'(x)\Delta x \\ e^{-i\alpha(x+\Delta x)} &\approx e^{-i\alpha(x)} (1 - i\nabla\alpha(x)\Delta x) \end{aligned}$$

we get transformation rule for electromagnetic vector potential

$A'(x) = A(x) + \nabla\alpha(x)$ or, in components, $A'_\mu(x) = A_\mu(x) + \dfrac{\partial\alpha(x)}{\partial x^\mu}$

Electrodynamics. Abelian prototype of all gauge theories. II

- Differential $F = (F_{\mu\nu}) = \mathrm{d}A$ of 1-form A is identified with electromagnetic field strength
- Replacing partial by covariant derivatives

$$\partial_\mu \to D_\mu = \partial_\mu - iA_\mu(x)$$

provides gauge invariance of (Schrödinger or Dirac) equations for field $\psi(x)$

- Finally, evolution equations for gauge field $A(x)$ should be added. In the case of electromagnetics these are Maxwell's equations:

$$\begin{aligned} \mathrm{d}F &= 0 \qquad \textit{first pair} \\ \mathrm{d}\star F &= 0 \qquad \textit{second pair} \end{aligned}$$

$\star$ is Hodge conjugation (Hodge star operator)

Non-Abelian Gauge Theories In Continuous Space-Time

- $u(x) \in W = \Gamma^X$ — Γ is non-Abelian Lie group
- $P(x, x + \Delta x) \approx 1 + A_\mu(x)\Delta x^\mu$ — approximation of parallel transport via Lie-algebra-valued 1-form
- $A'_\mu(x) = u(x)^{-1} A_\mu(x) u(x) + u(x)^{-1} \frac{\partial u(x)}{\partial x^\mu}$ — transformation rule
- $F = dA + [A \wedge A]$ — curvature form (= forces in physics)
  $F \equiv 0$ for trivial connection $\widetilde{A}_\mu(x) = u_0(x)^{-1} \frac{\partial u_0(x)}{\partial x^\mu}$
- $L_{YM} = \mathrm{Tr}\,[F \wedge \star F]$ — typical (Yang–Mills) invariant Lagrangian determining evolution of gauge field

Instructive note:
Discrete approximation of L_{YM} is proportional to $\sum_f \sigma(\gamma_f)$

- $\sigma = 2 \dim U - (\chi_U + \chi_{U^\dagger})$
- χ_U is character of fundamental representation U of Γ
- $\gamma_f \in \Gamma$ is holonomy around a face (cycle) of lattice in X

Approximation of Discrete Process by Continuous Physical Law: Heat Equation from Bernoulli Trials

$\{-,+\}$ — possible outcomes of single trial

$p_- = p,\ p_+ = q$ — probabilities of outcomes $(p+q=1)$

$n_-,\ n_+$ — numbers of outcomes in $t = n_- + n_+$ trials

Probability of separate history

$$P(n_-, n_+) = \frac{(n_- + n_+)!}{n_-!n_+!} p^{n_-} q^{n_+}$$

"space" *"time"* *"velocity" in limits* $-1 \le v \le 1$

$$x = n_+ - n_-,\ t = n_- + n_+,\ v = p - q, \quad \xrightarrow{\text{Stirling's approximation}}$$

$$P(x,t) \approx \widetilde{P}(x,t) = \frac{1}{\sqrt{1-v^2}} \sqrt{\frac{2}{\pi t}} \exp\left\{ -\frac{1}{2t} \left(\frac{x - vt}{\sqrt{1-v^2}} \right)^2 \right\}$$

– *fundamental solution* of heat (or diffusion or Fokker-Planck) equation

$$\frac{\partial \widetilde{P}(x,t)}{\partial t} + v \frac{\partial \widetilde{P}(x,t)}{\partial x} = \frac{(1-v^2)}{2} \frac{\partial^2 \widetilde{P}(x,t)}{\partial x^2}$$

Artifacts of Approximation

Problem from mechanics: find extremal trajectories connecting points $(0,0)$ and (X,T)

Our version of "least action principle" is maximum probability of trajectories

Probability of trajectory $(0,0) \to (x,t) \to (X,T)$

$$P_{(0,0)\to(x,t)\to(X,T)} = \frac{P(x,t)P(X-x,T-t)}{P(X,T)} \quad \text{(conditional probability)}$$

$$= \frac{t!(T-t)!\left(\frac{T-X}{2}\right)!\left(\frac{T+X}{2}\right)!}{\left(\frac{t-x}{2}\right)!\left(\frac{t+x}{2}\right)!\left(\frac{T-t}{2}-\frac{X-x}{2}\right)!\left(\frac{T-t}{2}+\frac{X-x}{2}\right)!T!}$$

⋆ Several trajectories with the same maximum probability

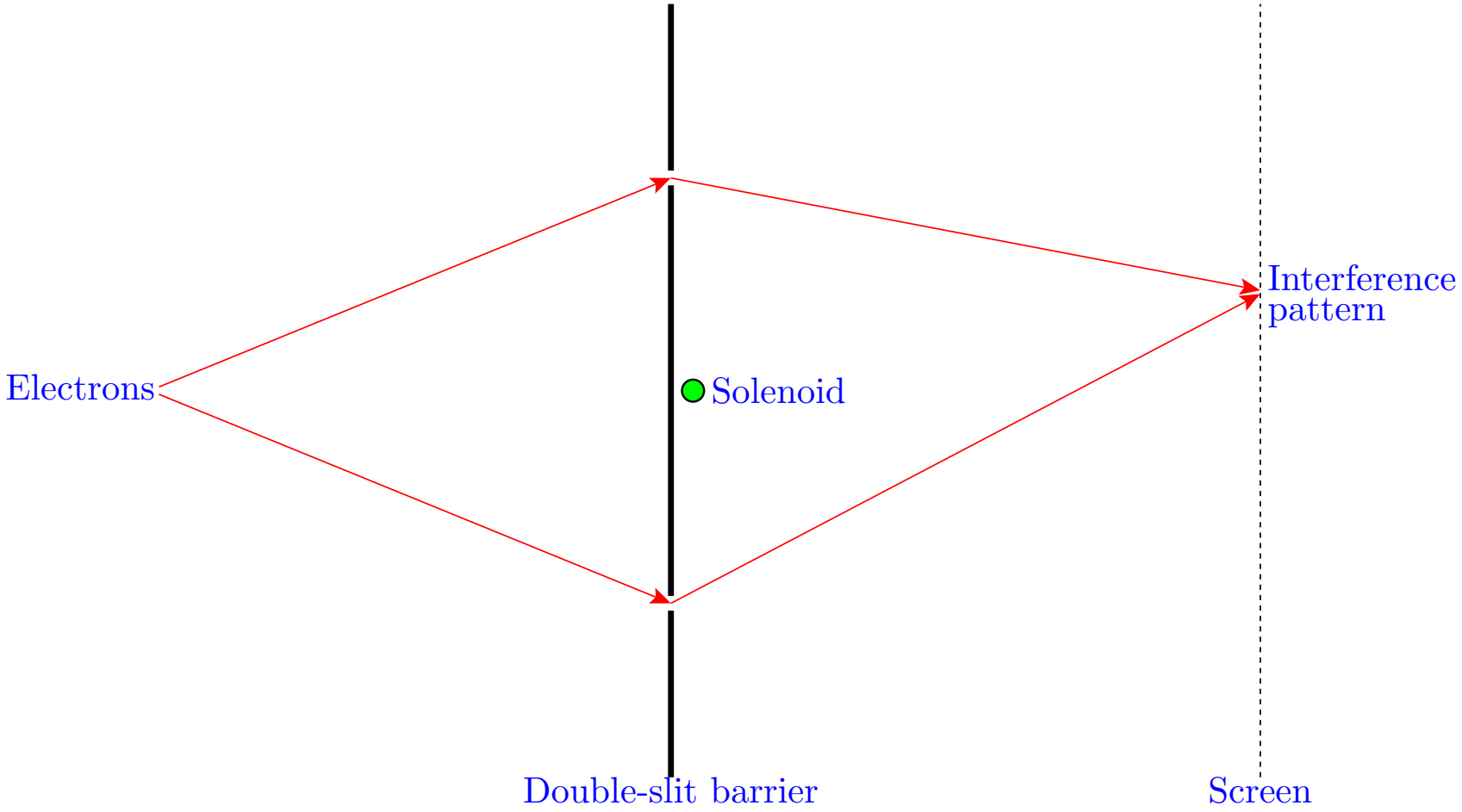
⋆ No dependence on v

$$\widetilde{P}_{(0,0)\to(x,t)\to(X,T)} = \frac{T}{\sqrt{\frac{\pi}{2}(1-v^2)tT(T-t)}} \exp\left\{-\frac{(Xt-xT)^2}{2(1-v^2)tT(T-t)}\right\}$$

- Deterministic trajectory of maximum probability – straight line $x = \frac{X}{T}t$
- Artificial dependence on v

Interplay Between Quantum Behavior and Gauge Connection. Aharonov – Bohm Effect

Shift of interference pattern in spite of absence of electromagnetic field outside the solenoid



Quantization Based On Finite Group

Feynman's path amplitude

in discrete time decomposes into product of group elements

$$A_{\mathrm{U}(1)} = \exp(iS) = \exp\left(i\int L dt\right) \longrightarrow e^{iL_{0,1}} \ldots e^{iL_{t-1,t}} \ldots e^{iL_{T-1,T}}$$

Let us interpret $P(t-1,t) = e^{iL_{t-1,t}}$ as $\mathrm{U}(1)$-connection

Now let us replace $A_{\mathrm{U}(1)}$

by the following parallel transport

$$A_\Gamma = \rho\left(\alpha_{0,1}\right) \ldots \rho\left(\alpha_{t-1,t}\right) \ldots \rho\left(\alpha_{T-1,T}\right)$$

- $\Gamma = \{\gamma_0 = 1, \ldots, \gamma_{M-1}\}$ — some M-element finite group
- $\alpha_{t-1,t} \in \Gamma$
- ρ — d-dimensional unitary representation of Γ on space Ψ

Representations Of Finite Groups. Main properties

- All linear representations are unitary
- Any unitary representation ρ is determined uniquely by its character defined as

$$\chi_\rho(\alpha) = \mathrm{Tr}\rho(\alpha), \quad \alpha \in \Gamma$$

- All values of χ_ρ and eigenvalues of ρ are elements of the ring $\mathbb{A}$ of algebraic integers, moreover eigenvalues are roots of unity
- If all different irreducible representations of Γ are $\rho_1, \cdots, \rho_i, \cdots, \rho_h$ and $d_i = \dim \rho_i$, $M = |\Gamma|$ then

$$\sum_{i=1}^{h} d_i^2 = M \text{ and any } d_i \text{ divides } M: \quad d_i | M$$

- Any function $\varphi(\alpha)$ depending only on conjugacy classes of Γ (i.e., $\varphi\left(\beta^{-1}\alpha\beta\right) = \varphi\left(\alpha\right)$) (called central or class function) is linear combination of characters $\chi_{\rho_1}, \cdots, \chi_{\rho_h}$

Amplitudes And Probabilities

Amplitude at point of observation (x, T)

$$A = \sum_{k=0}^{M-1} n_k \rho(\gamma_k)\psi \qquad \gamma_k \in \Gamma,\ \psi \in \Psi$$

n_k — non-negative integers (numbers of γ_k-valued paths)

Square of amplitude

$$\begin{aligned}\langle A\psi|A\psi\rangle &= \sum_{k=0}^{M-1} n_k^2 |\psi|^2 + \sum_{\substack{\gamma_i,\gamma_k\in\Gamma \\ i<k}} n_i n_k \left\langle \psi \left| \rho\left(\gamma_i^{-1}\gamma_k\right) + \rho^\dagger\left(\gamma_i^{-1}\gamma_k\right) \right| \psi \right\rangle \\ &= \sum_{k=0}^{M-1} N_k(n_0, \cdots, n_{M-1}) \left\langle \psi \left| \rho(\gamma_k) + \rho^\dagger(\gamma_k) \right| \psi \right\rangle\end{aligned}$$

$N_k(n_0, \cdots, n_{M-1})$ — 2nd-order integer polynomials

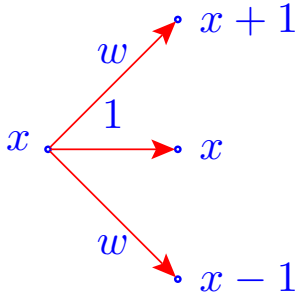
All within algebraic integers except of "probabilities" requiring quotient field of $\mathbb{A}$

Simple Model Inspired By Free Particle

In quantum mechanics transitions between arbitrary states are possible since $\exp\left(\frac{i}{\hbar}S\right)$ never vanishes, but we shall consider models with restricted sets of possible transitions

Lagrangian of free particle $L = \frac{m\dot{x}^2}{2}$

Rule



$$e^{\frac{i}{\hbar}\frac{m\{(x+1)-x\}^2}{2}} = e^{i\frac{m}{2\hbar}}$$

$$e^{\frac{i}{\hbar}\frac{m(x-x)^2}{2}} = 1 \qquad e^{i\frac{m}{2\hbar}} = e^{2\pi i\alpha} \rightsquigarrow w = e^{\frac{2\pi i}{M}}$$

$$e^{\frac{i}{\hbar}\frac{m\{(x-1)-x\}^2}{2}} = e^{i\frac{m}{2\hbar}}$$

Sum amplitude over all paths $(0,0) \longrightarrow (x,t)$

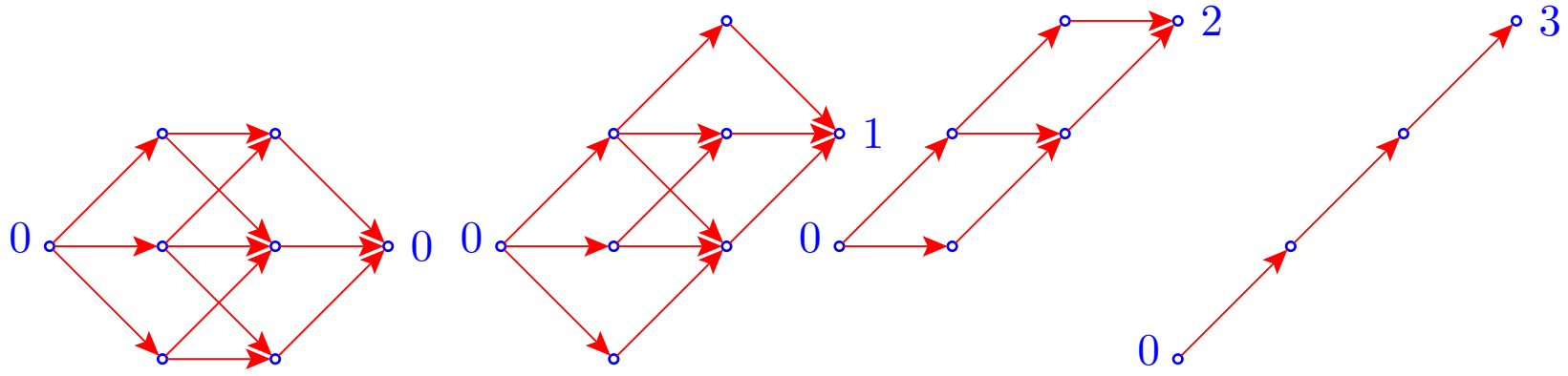
$$A_x^t(w) = \sum_{\tau=0}^{t} \frac{\tau!}{\left(\frac{\tau-x}{2}\right)!\left(\frac{\tau+x}{2}\right)!} \times \frac{t!}{\tau!\,(t-\tau)!}\, w^\tau \quad \left\{\times p^{\frac{\tau-x}{2}} q^{\frac{\tau+x}{2}} h^{t-\tau}\right\}$$

$$x \in [-t,t] = -t, -t+1, \ldots, -1, 0, 1, \ldots, t-1, t$$

Searching Destructive Interference

Conditions for destructive interference: $w \in \mathbb{Z}_M \bigwedge A^t_x(w) = 0$

All paths in 3 time steps



Number of paths	7	6	3	1
Amplitude	$A^3_0 = 1 + 6w^2$	$A^3_{\pm 1} = 3w + 3w^3$	$A^3_{\pm 2} = 3w^2$	$A^3_{\pm 3} = w^3$

It follows from $A^3_{\pm 1} = 0$ that w must be 4th root of unity:

$$A^3_{\pm 1} = 0 \Rightarrow w^2 + 1 = 0 \Rightarrow w = \pm i = e^{\frac{2\pi i}{4} + k\pi i} \qquad \Longrightarrow \qquad w \in \mathbb{Z}_4$$

Interference From Two Sources. Group $\mathbb{Z}_4$

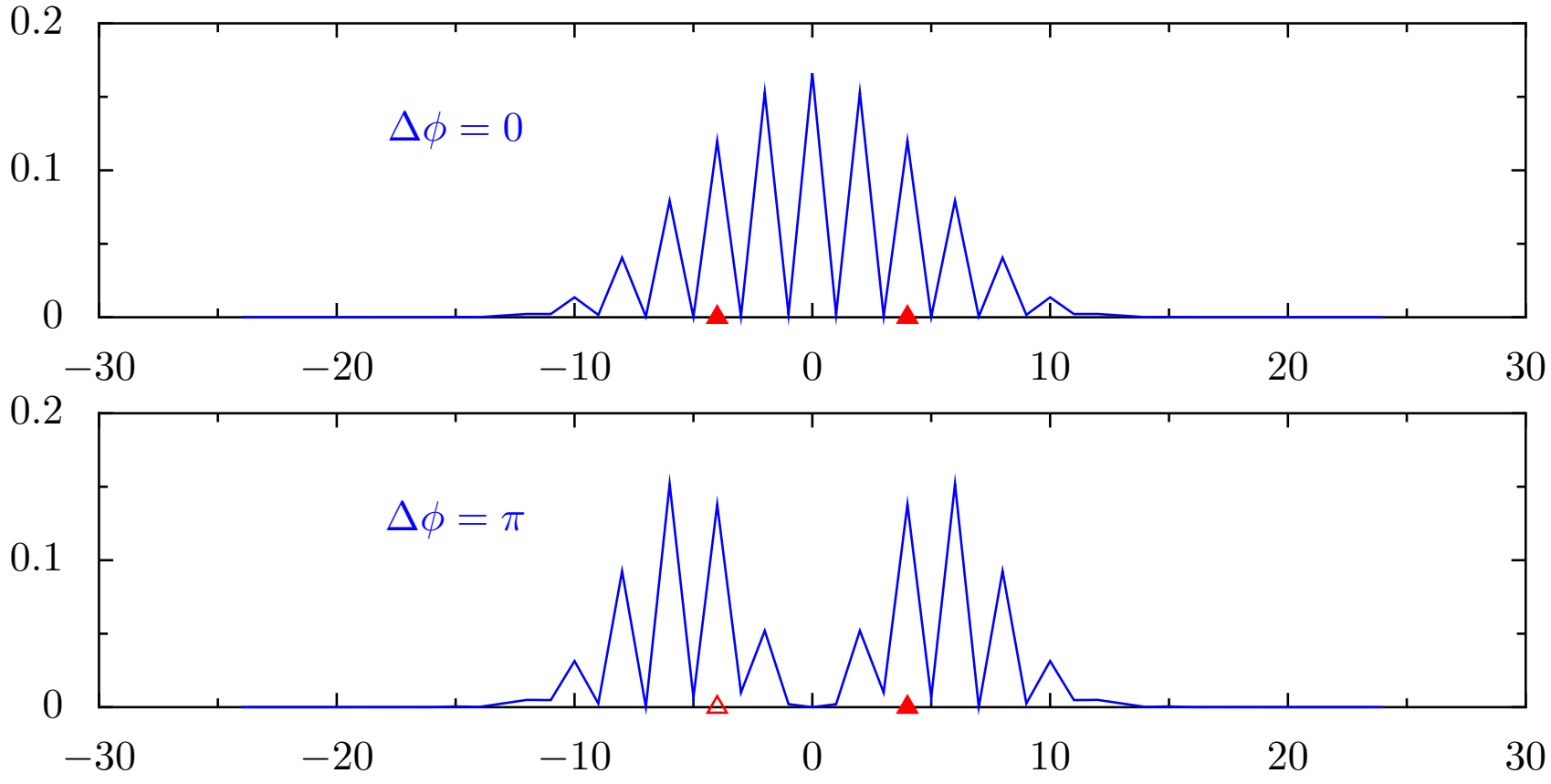
Space $X = [-24, \ldots, 24]$

Source positions -4 and 4

Number of time steps $T = 20$

Phase difference between sources $\Delta\phi = \phi_4 - \phi_{-4}$

Normalized squared amplitudes ("probabilities")



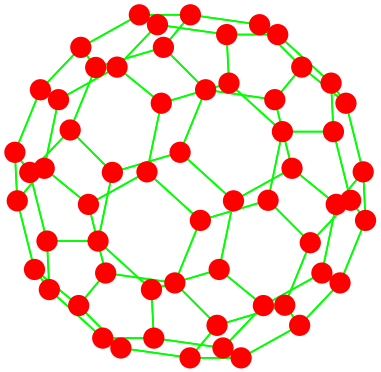
Generalization

Local Quantum Models On $k-$valent Graphs

- $X = \{x_1, \cdots, x_N\}$ is $k-$valent graph
- $V_i = \left\{x_i, x_{1,i}, \cdots, x_{k,i}\right\}$ is set of neighbors of x_i with x_i itself
- $E_i = \left\{e_{0,i}, e_{1,i}, \cdots, e_{k,i}\right\}$ is set of k adjacent edges
  $e_{m,i} = \left(x_i \to x_{m,i}\right)$ completed by edge $e_{0,i} = (x_i \to x_i)$
- $G = \mathrm{Aut}\,(X)$ acts transitively on vertices of X
- $G_{loc} = \mathrm{Stab}\,(x_i) \leq G$ is stabilizer of x_i
- $\Omega_i = \left\{\omega_{0,i}, \omega_{1,i}, \cdots, \omega_{h,i}\right\}$ is set of orbits of G_{loc} on E_i
- Γ is (representation of) some finite (quantizing) group
- Evolution rule $R : E_i \to \Gamma$ is Γ-valued function on E_i prescribing Γ-weights to one-time-step transitions from x_i to elements of V_i
  Natural requirement: R must be function on orbits Ω_i,
  i.e., $R\left(e_{m,i}g\right) = R\left(e_{m,i}\right)$ for $g \in G_{loc}$

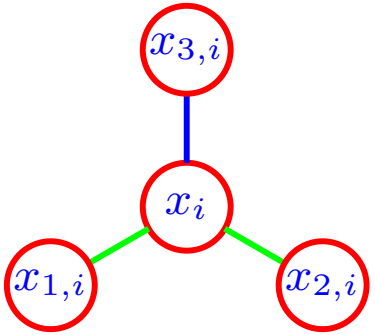
Illustration. Buckyball C_{60}

- $X = \{x_1, \cdots, x_{60}\}$



$G = \mathrm{Aut}\,(X) = \mathbb{Z}_2 \times \mathrm{Alt}(5)$

- $V_i = \{x_i,\ x_{1,i},\ x_{2,i},\ x_{3,i}\}$
  $E_i = \{e_{0,i}, e_{1,i}, e_{2,i}, e_{3,i}\}$



$G_{loc} = \mathrm{Stab}\,(x_i) = \mathbb{Z}_2$

- Orbits of G_i on E_i:
  $\Omega_i = \{\omega_{0,i} = \{e_{0,i}\}, \omega_{1,i} = \{e_{1,i}, e_{2,i}\}, \omega_{2,i} = \{e_{3,i}\}\}$

- Evolution rule R:
$$R\,(x_i \to x_i) = \gamma_0 \in \Gamma$$
$$R\,(x_i \to x_{1,i}) = R\,(x_i \to x_{2,i}) = \gamma_1 \in \Gamma$$
$$R\,(x_i \to x_{3,i}) = \gamma_2 \in \Gamma$$

Summary

- We suggest an algorithmic approach — based on discrete symmetry analysis and implemented in C — for construction and investigation of discrete dynamical models — deterministic, mesoscopic and quantum.
- Our approach is applicable to simulation of nanostructures with nontrivial symmetry properties. Important examples of such nanostructures are (hydro)carbon molecules like graphenes, fullerenes, etc.
- We formulate the gauge principle in the form most suitable for discrete and finite background.
- We propose a method — based on introduction of gauge connection of a special kind — for quantizing discrete systems.
- We construct simple models for studying properties of suggested quantization.