Quantum Computing for Modeling of Molecules and Materials

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Natural orbital properties for excited states

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UVIC

Quantum chemistry

Quantum many-body problem

- Eigenvalue problem

$$H\Psi = E\Psi$$

- Second quantization

$$\mathcal{H} = \sum_{ij} \left(t_{ij} \hat{c}_i^\dagger \hat{c}_i + \sum_{k\ell} V_{ijk\ell} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \right)$$

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Quantum chemistry

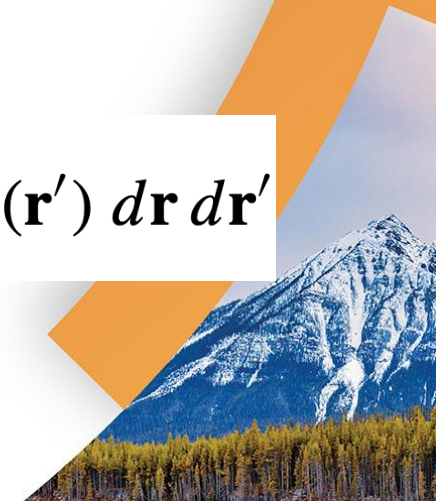
(Local) Basis functions

- One-electron integral

$$t_{ij} = \int \varphi_i^*(\mathbf{r}) \left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) \right] \varphi_j(\mathbf{r})\, d\mathbf{r}$$

- Two-electron integrals

$$V_{ijk\ell} = \frac{1}{2} \iint \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}') v_{\mathrm{ee}}(\mathbf{r} - \mathbf{r}') \varphi_k(\mathbf{r}) \varphi_\ell(\mathbf{r}')\, d\mathbf{r}\, d\mathbf{r}'$$



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Quantum chemistry

Density matrices

- Density matrix
  - Mixed, pure, ensemble
  - Normalization

$$\rho = \sum_k \eta_k |\psi_k\rangle\langle\psi_k|$$

$$0 \leq \eta_k \leq 1$$

Quantum chemistry

Density matrices (mixed basis)

- One-body reduced density matrix

$$\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j|$$

$$\rho_{ij} = \langle \Psi | \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} | \Psi \rangle$$

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Quantum chemistry

Natural orbitals

- Diagonalization of the density matrix
  - Löwdin (1955)

$$\rho^{(\alpha)} \rightarrow \{\varepsilon_k^{(\alpha)}\}, \{\Phi_k^{(\alpha)}\}$$

Truncation

- Density matrix of a subsystem
  - Truncation of small weights

$$\hat{\rho} = \psi\psi^{\dagger} = \begin{pmatrix} 0.98 & 0 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & 0 & 0 \\ 0 & 0 & \cancel{0.0005} & 0 & 0 \\ 0 & 0 & 0 & \cancel{0.0003} & 0 \\ 0 & 0 & 0 & 0 & \cancel{0.0002} \end{pmatrix}$$

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Bundled density matrices

Independent density matrices

- No restrictions on types

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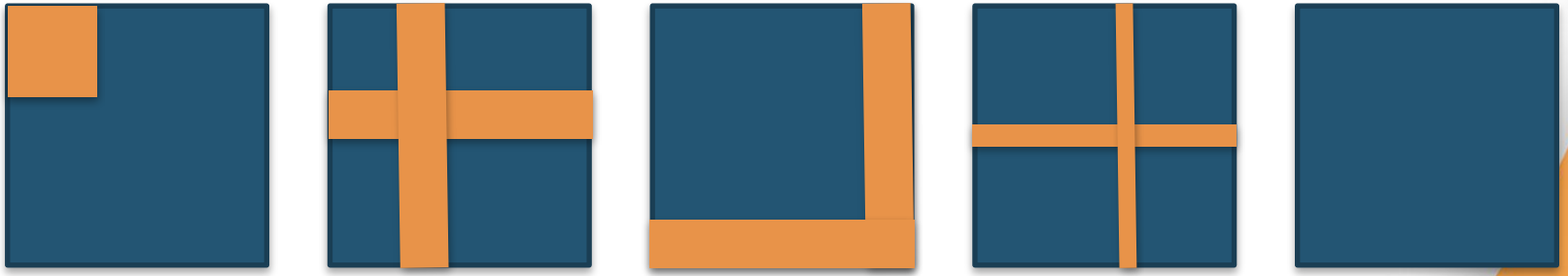

1 2 3 4 5

Formal definitions

Density matrices

- Expectation values

$$E = \mathrm{Tr}(\rho H) \equiv \sum_k \langle k|\rho H|k\rangle$$

- Energy differences

$$\Delta E_{\alpha\beta} = \mathrm{Tr}\left((\rho^{(\alpha)} - \rho^{(\beta)})H\right)$$

- Truncation error

$$\sum_{i=1}^{M} \rho_i^{(\alpha)} - \sum_{i=1}^{m} \rho_i^{(\alpha)} \equiv \delta_{m;\gamma}^{(\alpha)}$$

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Relationship between density matrices

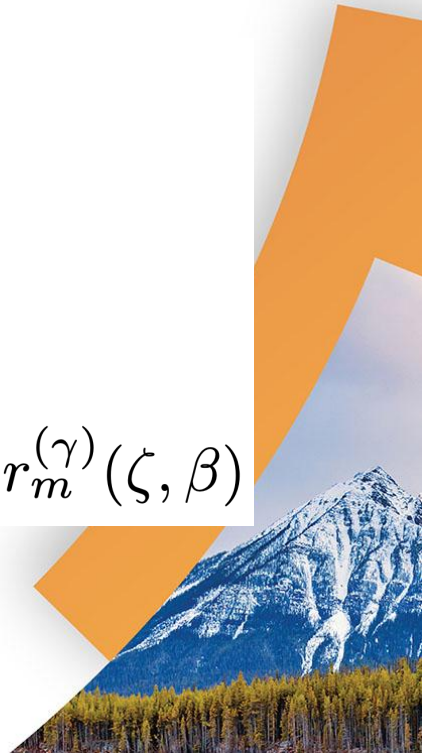
$$r_m^{(\gamma)}(\alpha,\beta) = |\delta_{m;\gamma}^{(\alpha)} - \delta_{m;\gamma}^{(\beta)}|$$

Metric distance:

1. $r_m^{(\gamma)}(\alpha,\alpha) = 0$
2. $r_m^{(\gamma)}(\alpha,\beta) \geq 0$
3. $r_m^{(\gamma)}(\alpha,\beta) = r_m^{(\gamma)}(\beta,\alpha)$
4. $r_m^{(\gamma)}(\alpha,\beta) \leq r_m^{(\gamma)}(\alpha,\zeta) + r_m^{(\gamma)}(\zeta,\beta)$

$$\Delta E_{\alpha\beta}^{(m)}$$

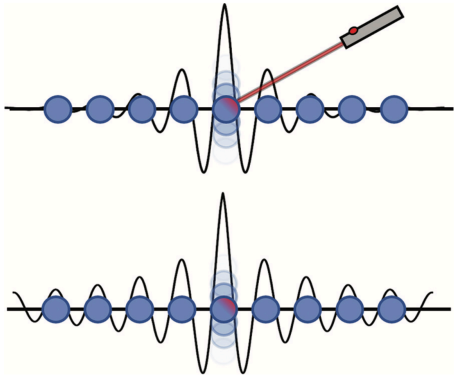
Also a metric distance (Local systems)



How local is nature? (Everything is local)

- Area law

- Kohn's principle of nearsightedness



$$\begin{cases} \exp(-x/\xi) & \text{gapped} \\ 1/x^{\gamma} & \text{gapless} \end{cases}$$

T.E. Baker, et. al., *Can. J. Phys.* **99**, 4 (2021)

ibid, arxiv: 1911.11566

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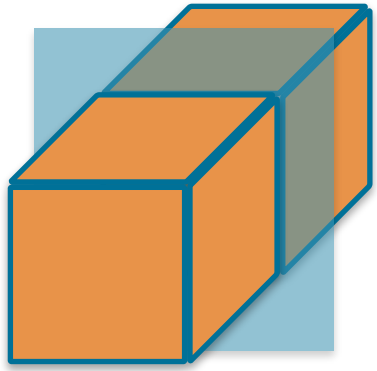
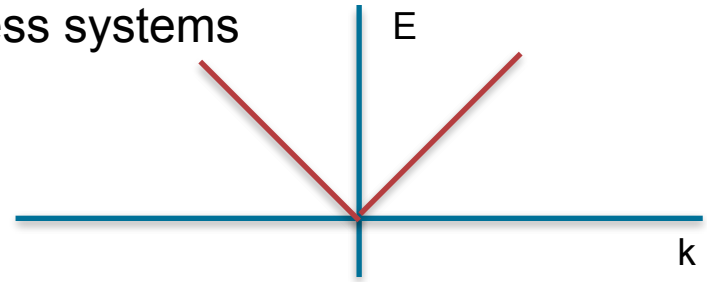
Entanglement

$$S = -\mathrm{Tr}(\rho \ln \rho)$$

- Good for volume law scaling systems



- Gapless systems



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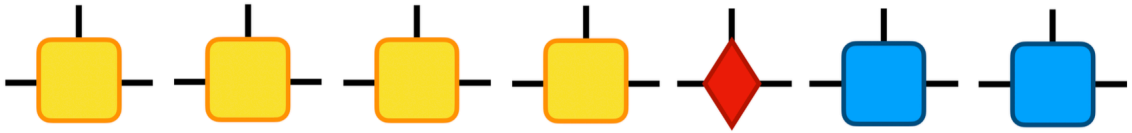
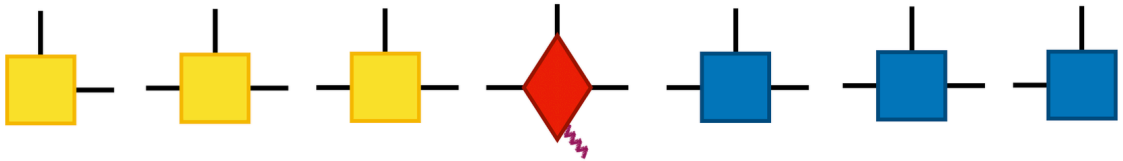
Entanglement renormalization

- Matrix product state (MPS)



T.E. Baker, *et. al.*, Can. J. Phys. **9**, 207 (2021)

- Bundled MPS



T.E. Baker, A. Foley, D. Sénéchal, arxiv: 2109.08181

Bundled matrix product states in DMRG

Direct solution of multiple excitations in a matrix product state with block Lanczos

Thomas E. Baker,[1,2] Alexandre Foley,[1] and David Sénéchal[1]

[1] *Institut quantique & Département de physique, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1 Canada*
[2] *Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom*

(Dated: September 20, 2021)

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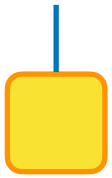
Efficient modeling of superconducting quantum circuits with tensor networks

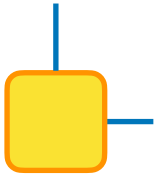
Agustin Di Paolo[1], Thomas E. Baker[1], Alexandre Foley[1], David Sénéchal[1] and Alexandre Blais[1,2]✉

We use a tensor network method to compute the low-energy excitations of a large-scale fluxonium qubit up to a desired accuracy. We employ this numerical technique to estimate the pure-dephasing coherence time of the fluxonium qubit due to charge noise and coherent quantum phase slips from first principles, finding an agreement with previously obtained experimental results. By developing an accurate single-mode theory that captures the details of the fluxonium device, we benchmark the results obtained with the tensor network for circuits spanning a Hilbert space as large as 15^{180}. Our algorithm is directly applicable to the wide variety of circuit-QED systems and may be a useful tool for scaling up superconducting

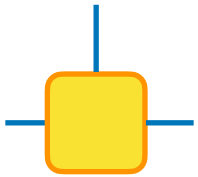
Easy to Read Diagrams



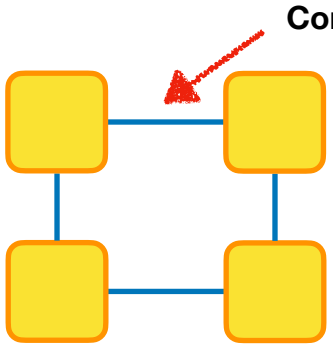
A^{μ}



$A^{\mu\nu}$

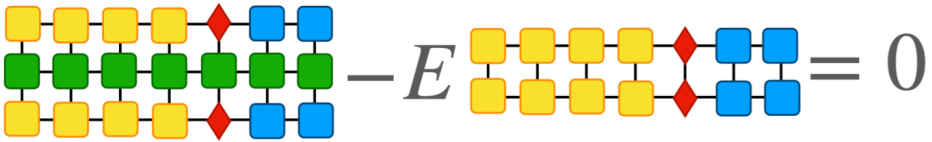


$A^{\mu\nu\gamma}$

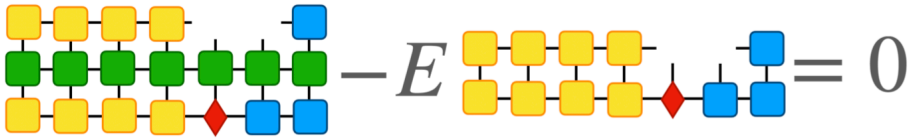


$\mathrm{Tr}(A^{\alpha\beta}A^{\beta\gamma}A^{\gamma\delta}A^{\delta\zeta})$

Density matrix renormalization group



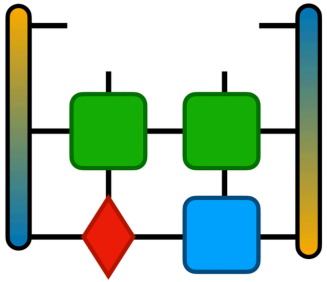
$$\frac{\partial^2}{\partial A^{*\sigma_i}_{a_{i-1}a_i} \partial A^{*\sigma_{i+1}}_{a_i a_{i+1}}} \Big(\langle \Psi | \mathcal{H} | \Psi \rangle - E \langle \Psi | \Psi \rangle \Big) = 0$$



T.E. Baker and M.P. Thompson, arxiv: 2019.03120

Density matrix renormalization group

1.

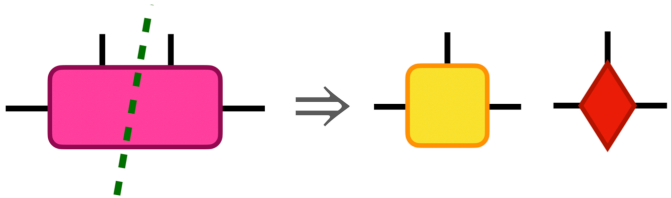


2.

$$|\psi_{n+1}\rangle = \mathcal{H}|\psi_n\rangle - \alpha_n|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle$$

$$\alpha_n = \langle\psi_n|\mathcal{H}|\psi_n\rangle \quad \text{and} \quad \beta_n^2 = \langle\psi_{n-1}|\psi_{n-1}\rangle$$

3.



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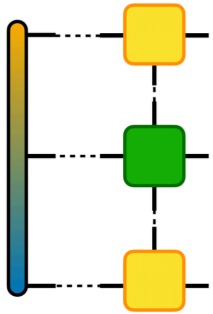

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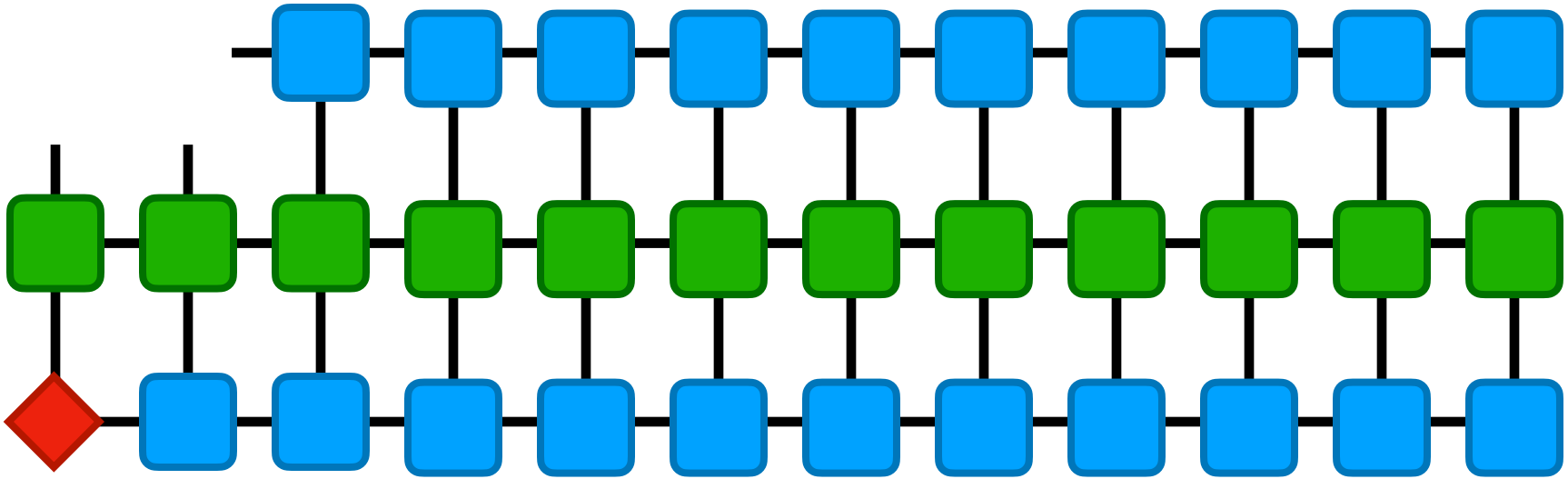
Density matrix renormalization group



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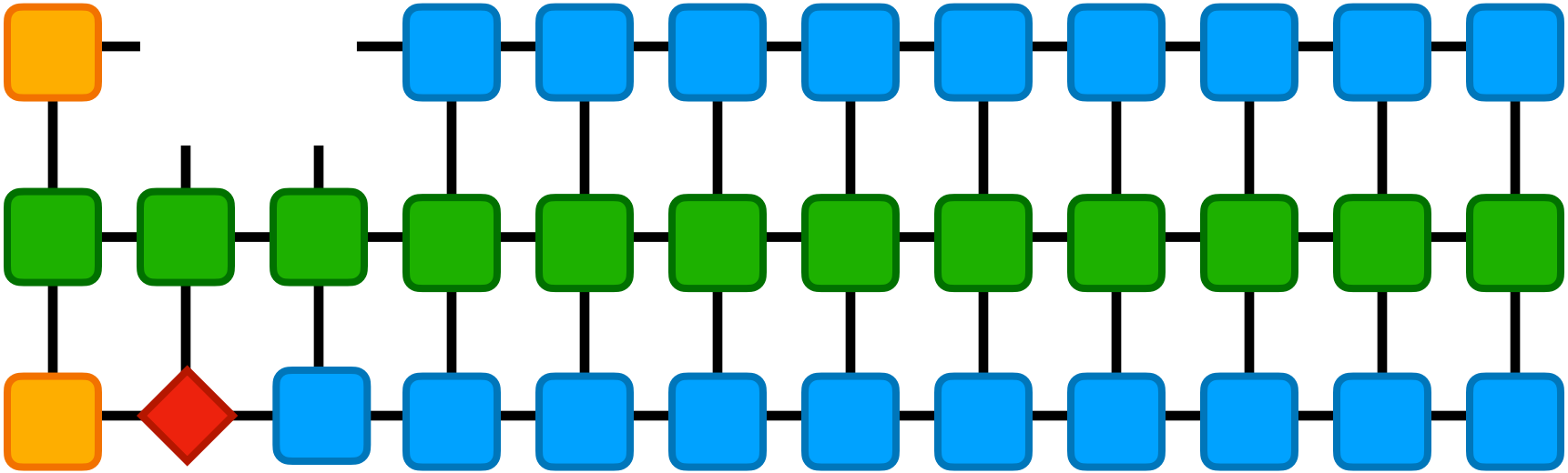

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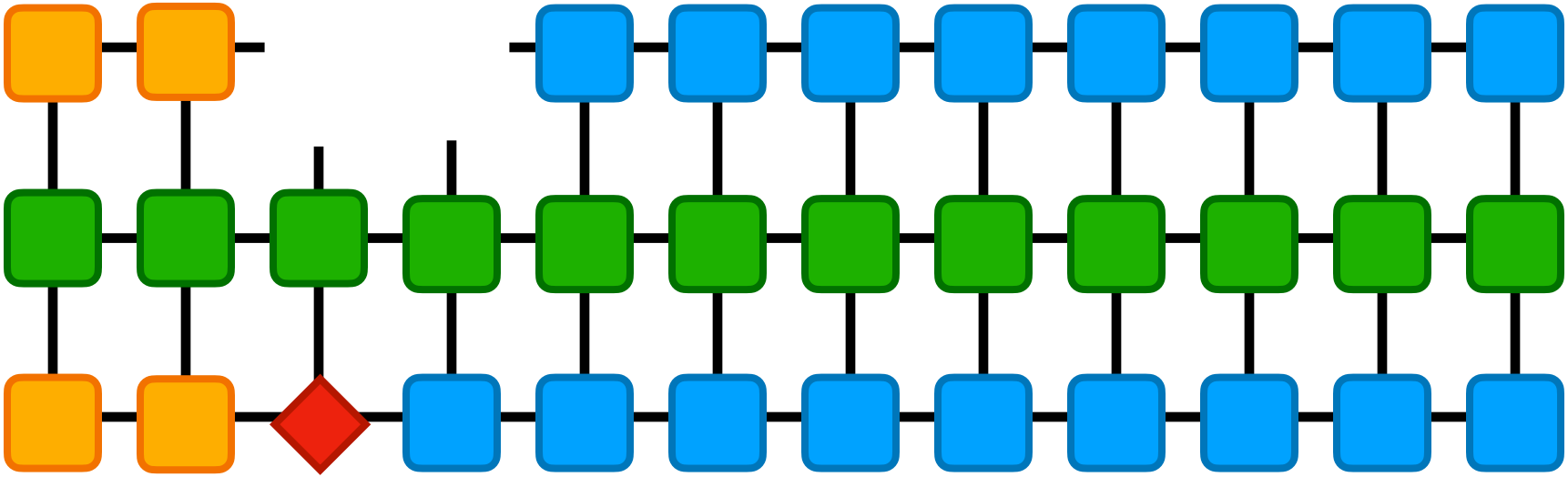

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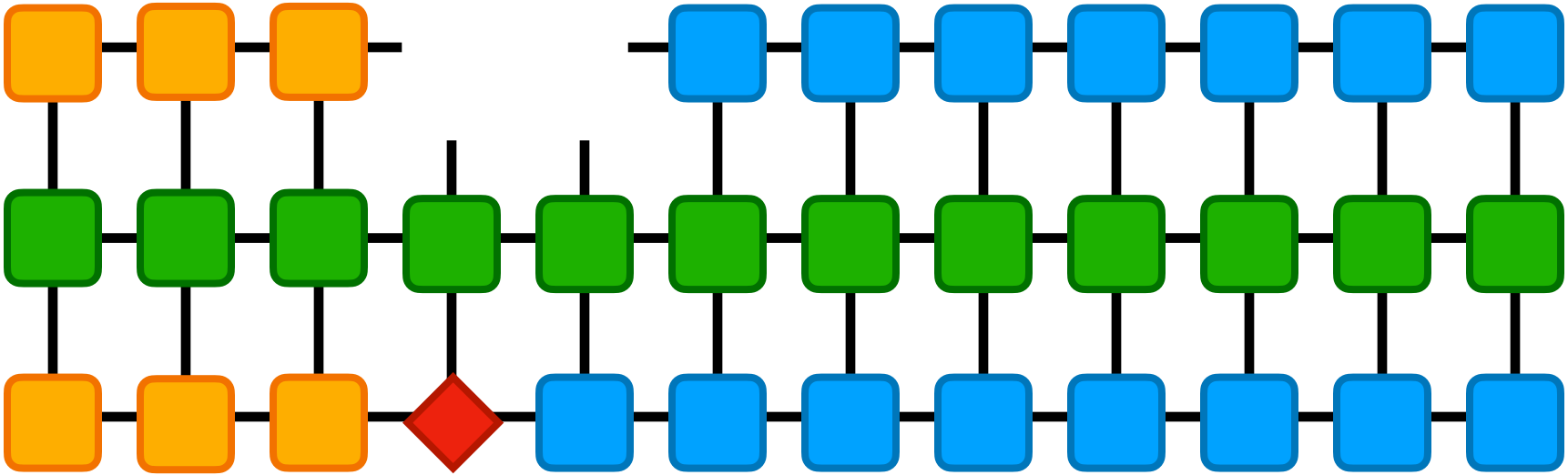

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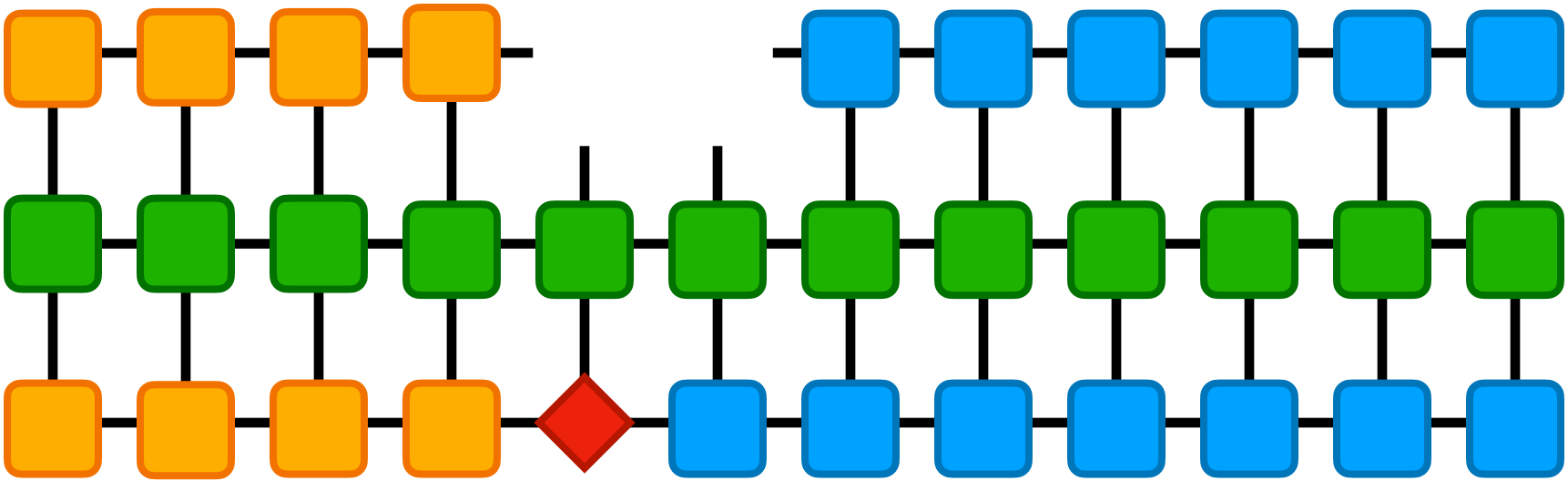

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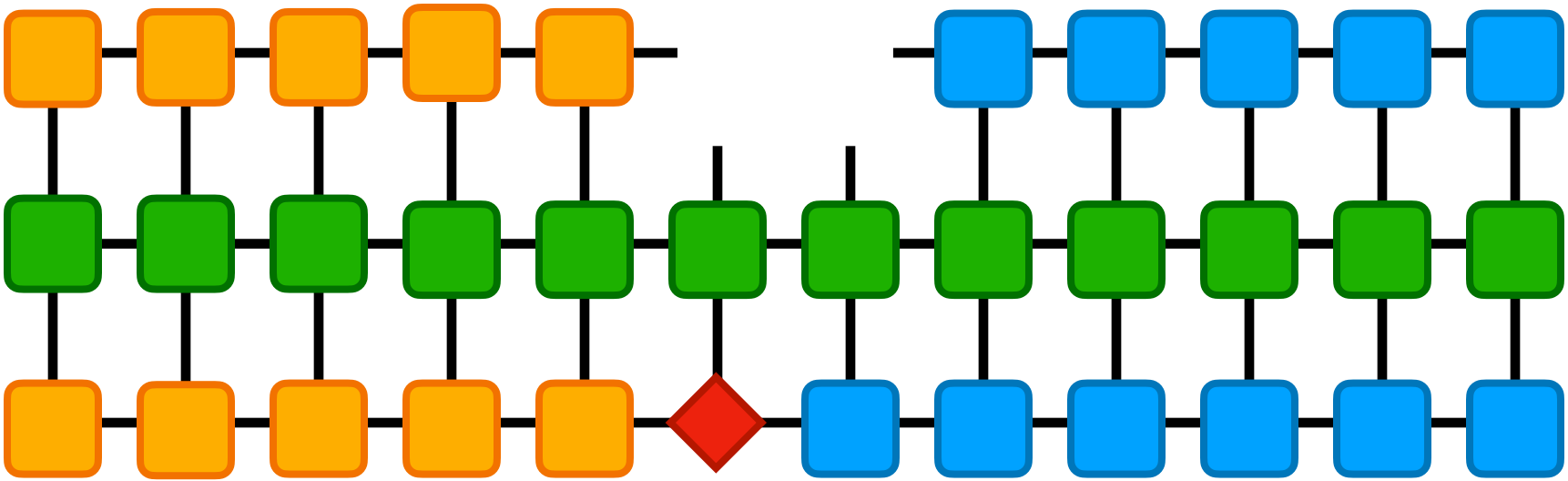

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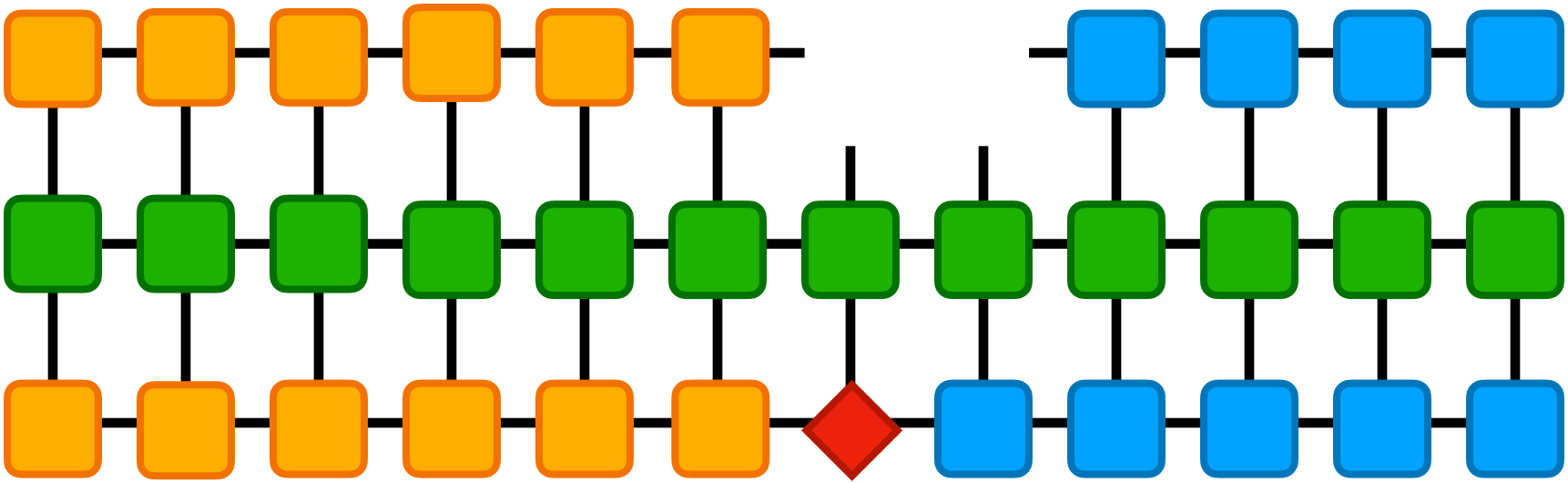

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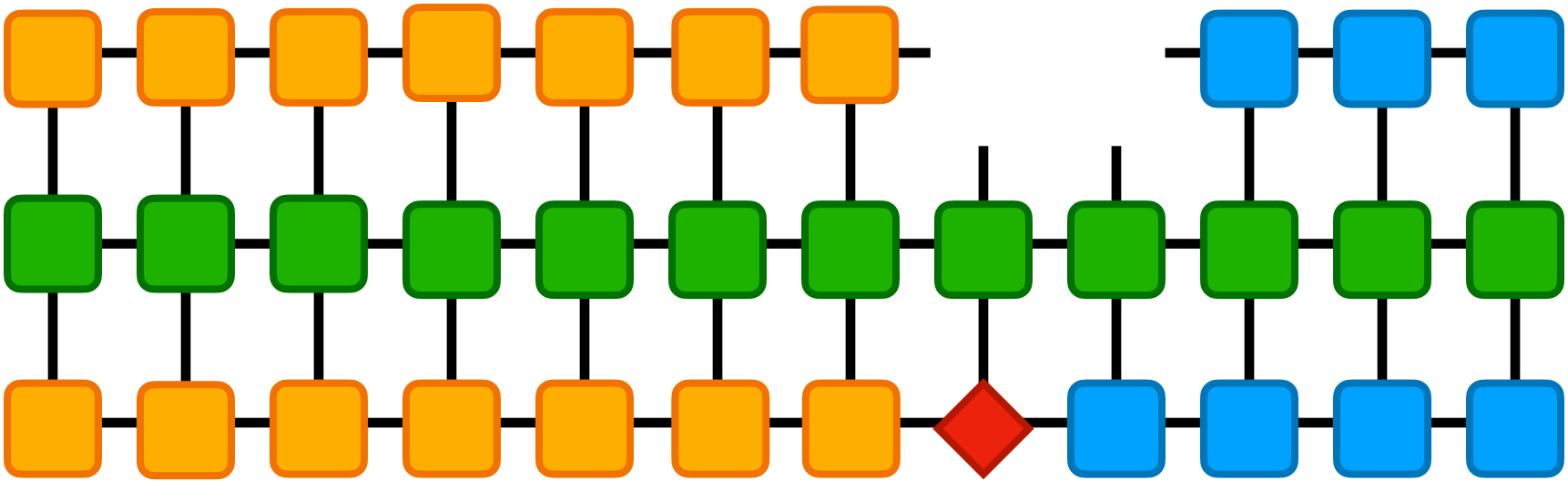

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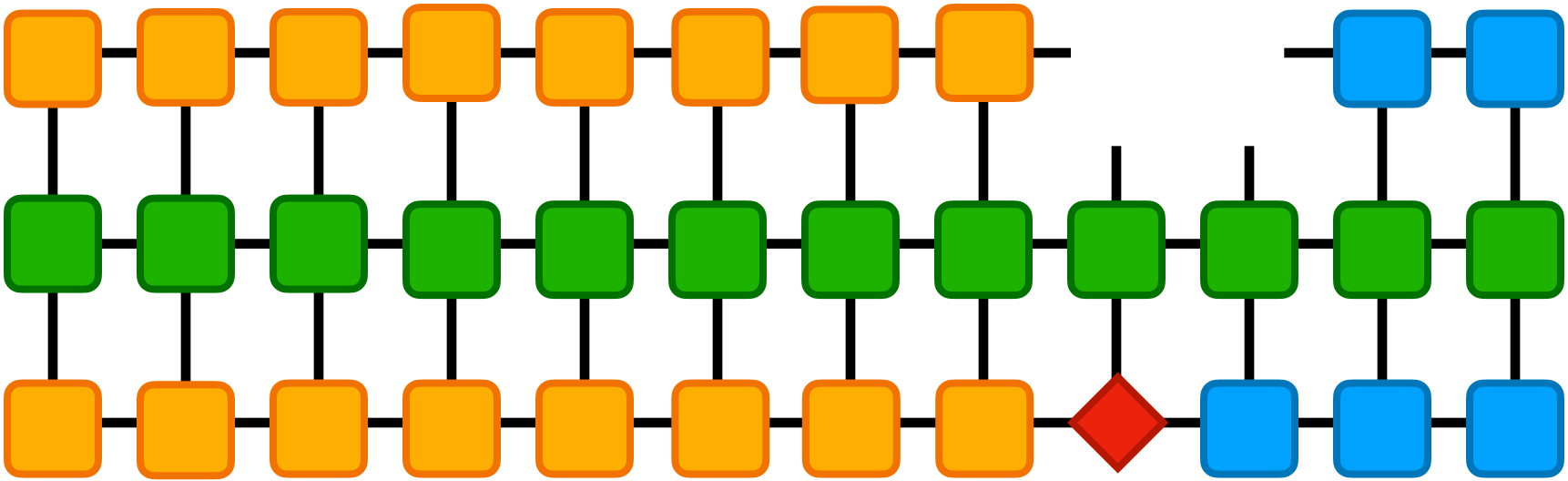

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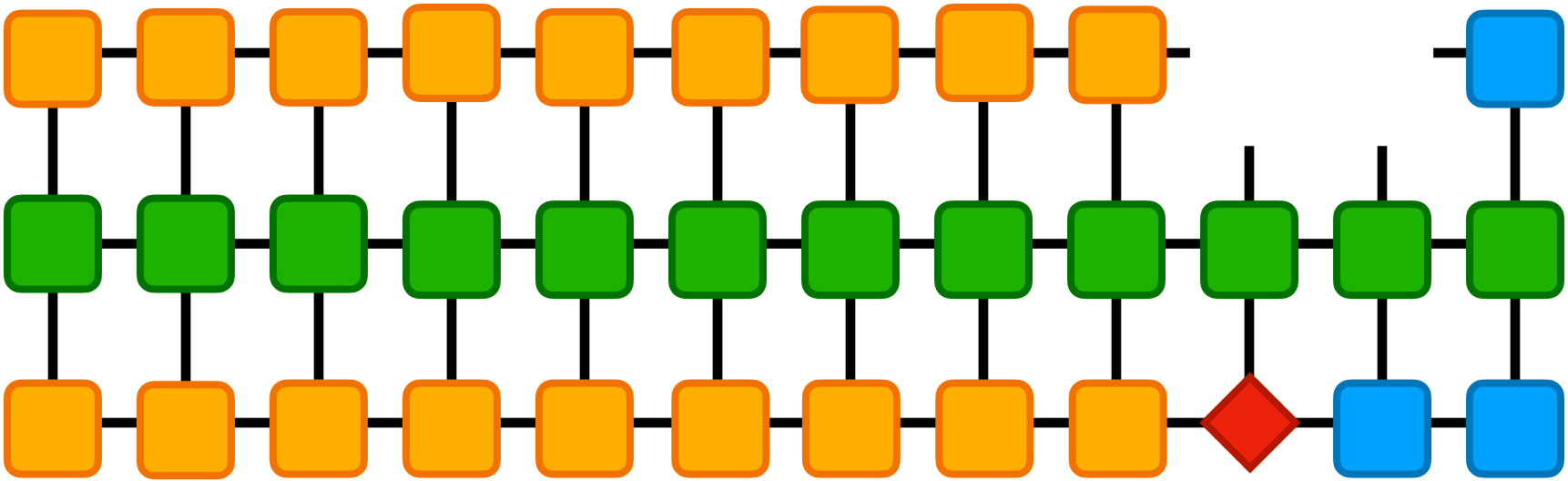

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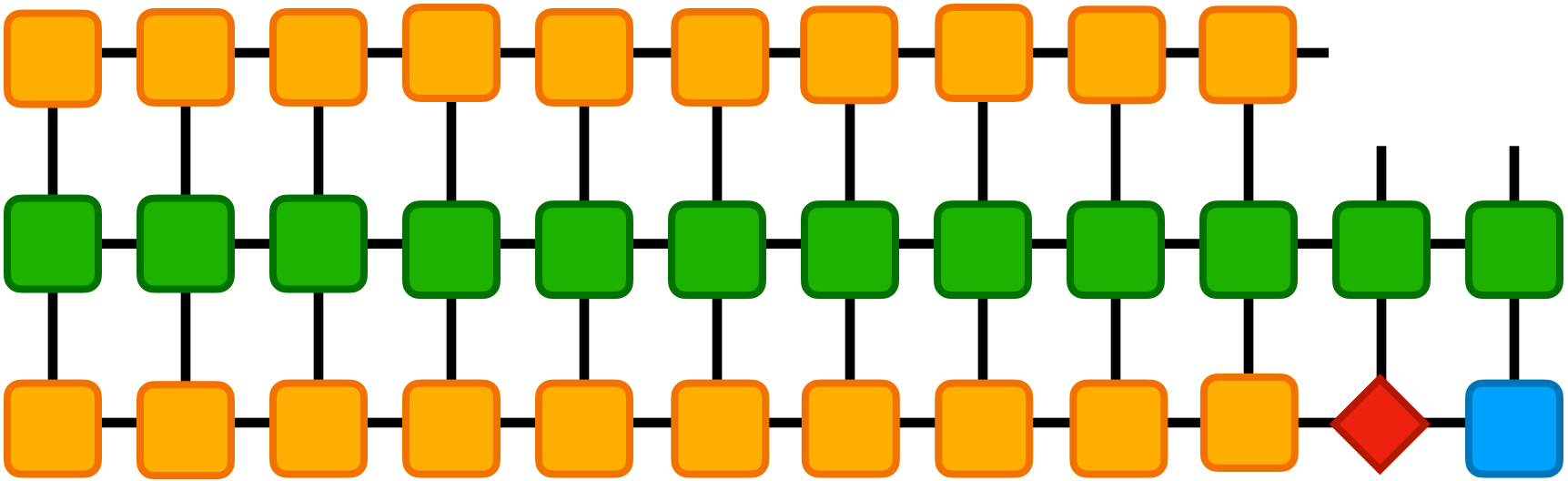

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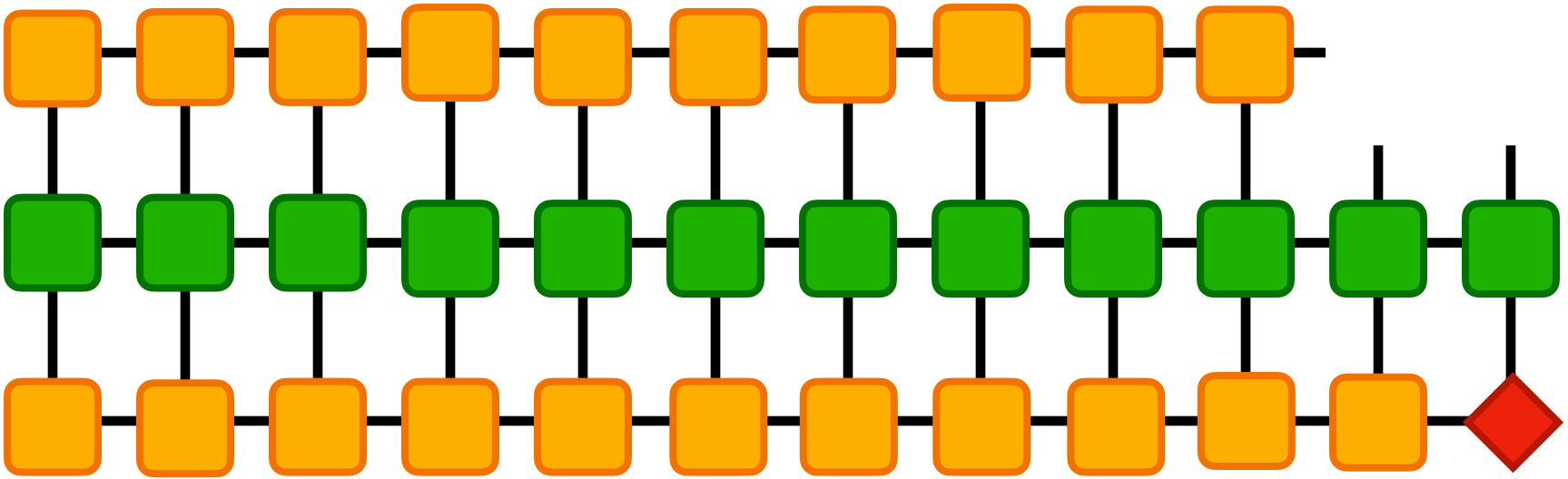

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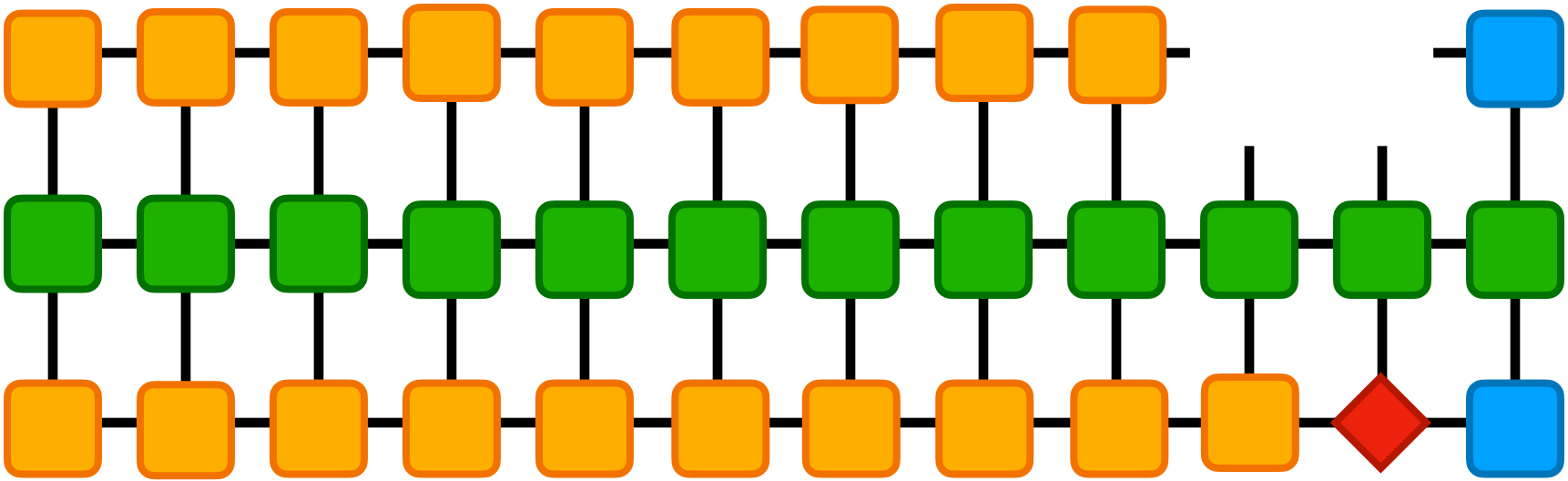

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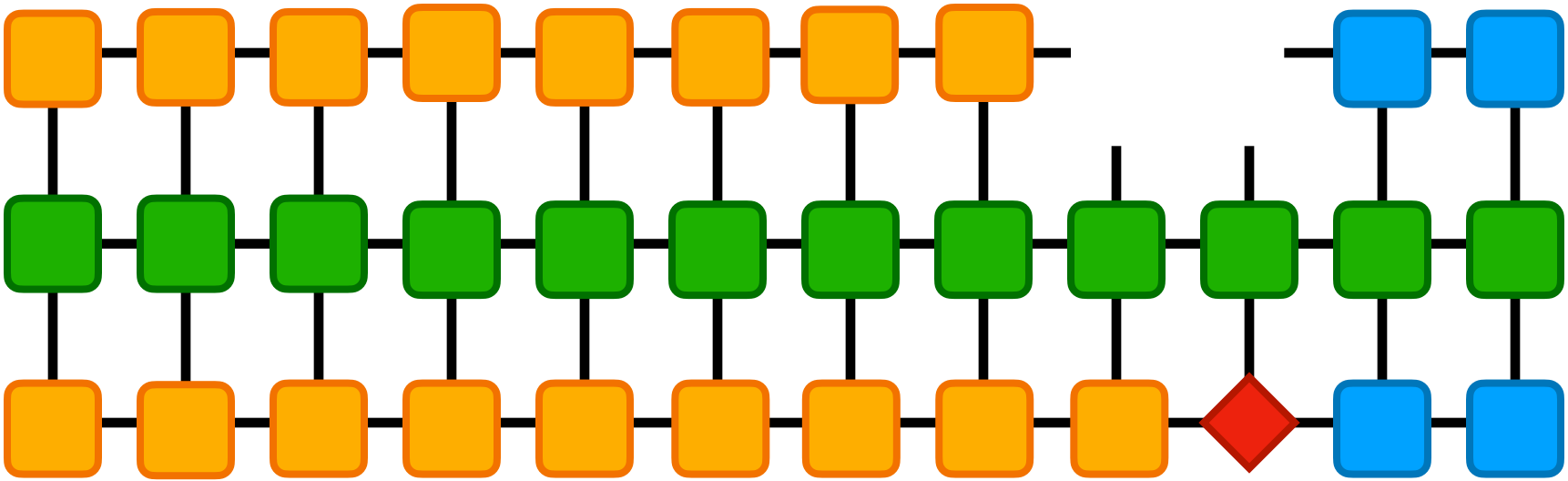

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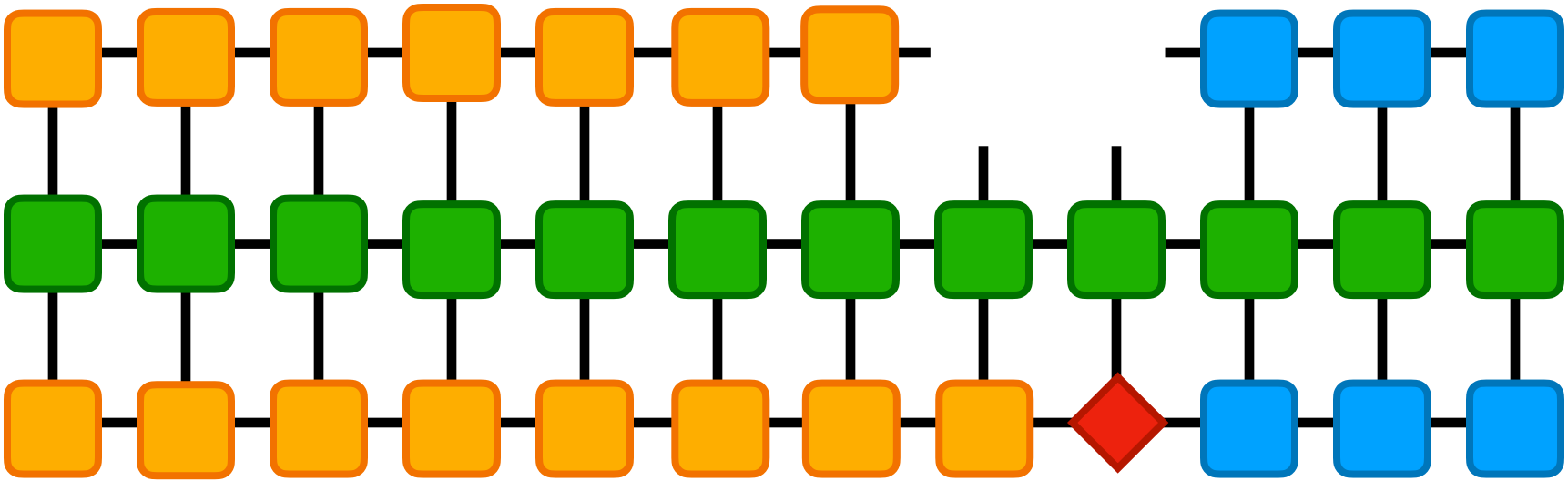

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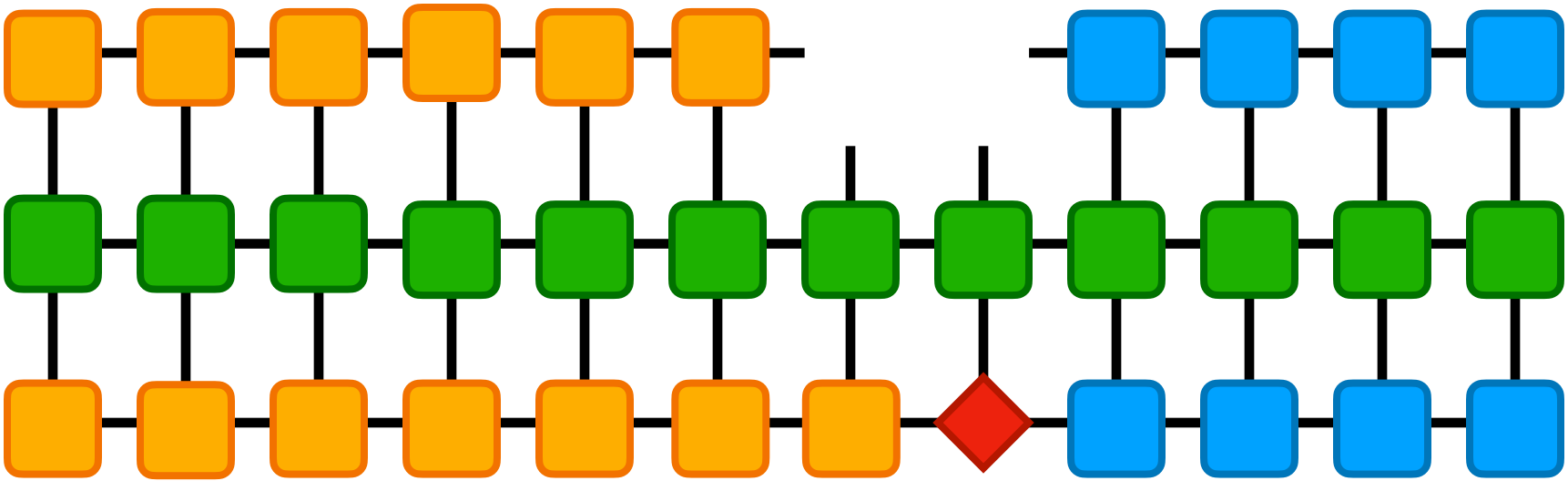

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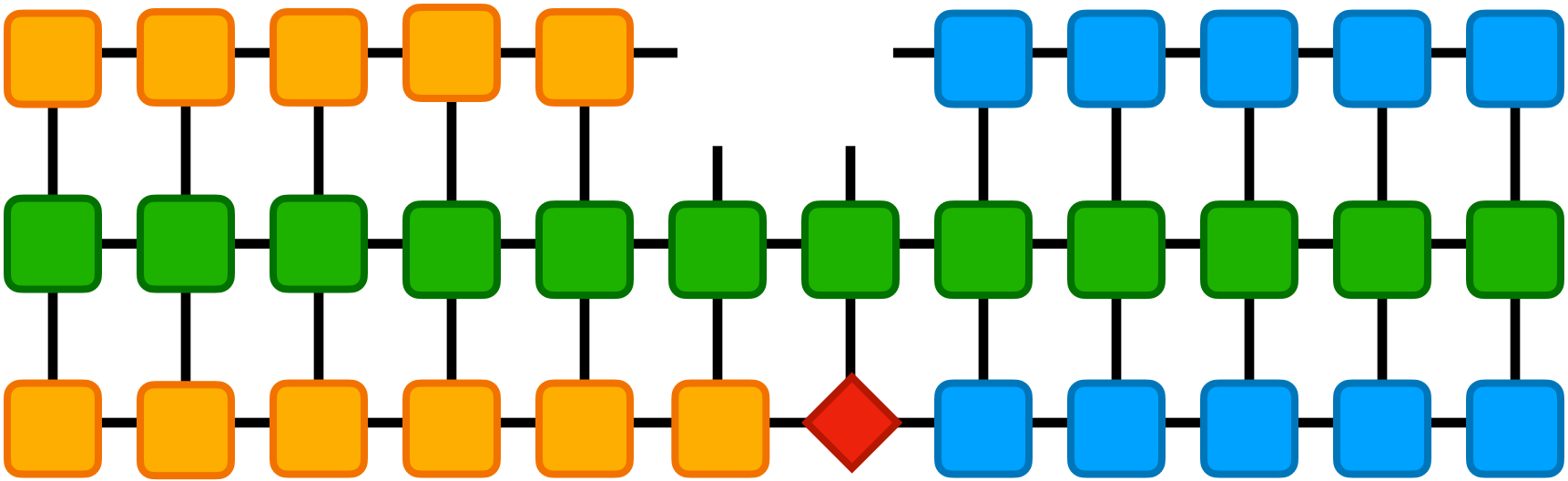

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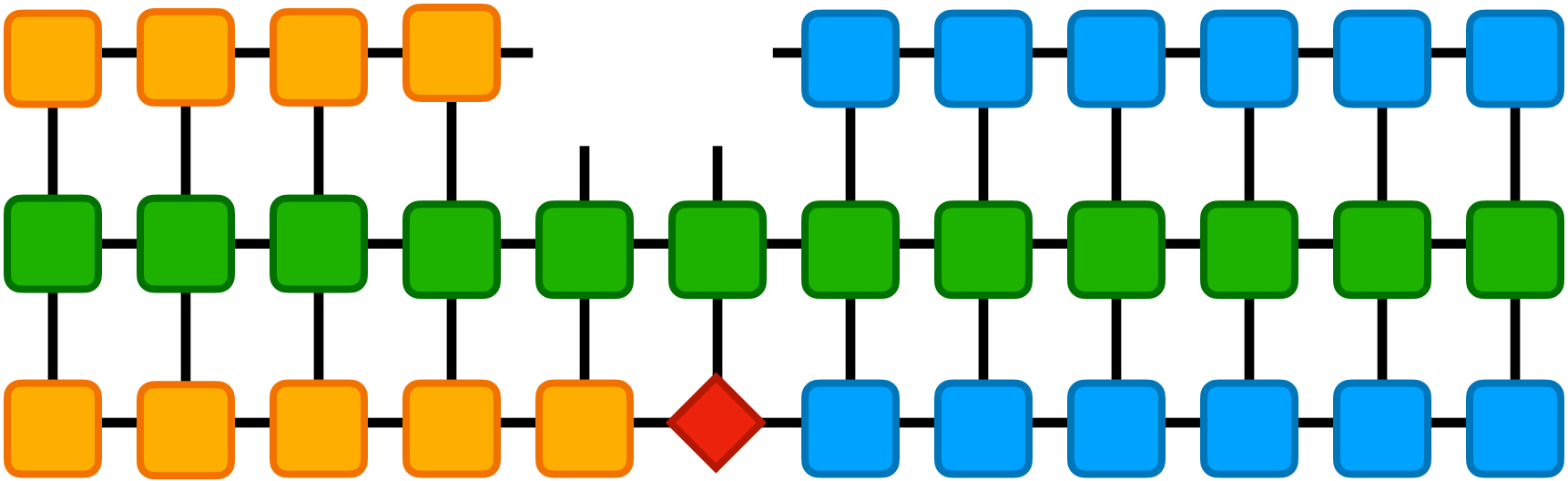

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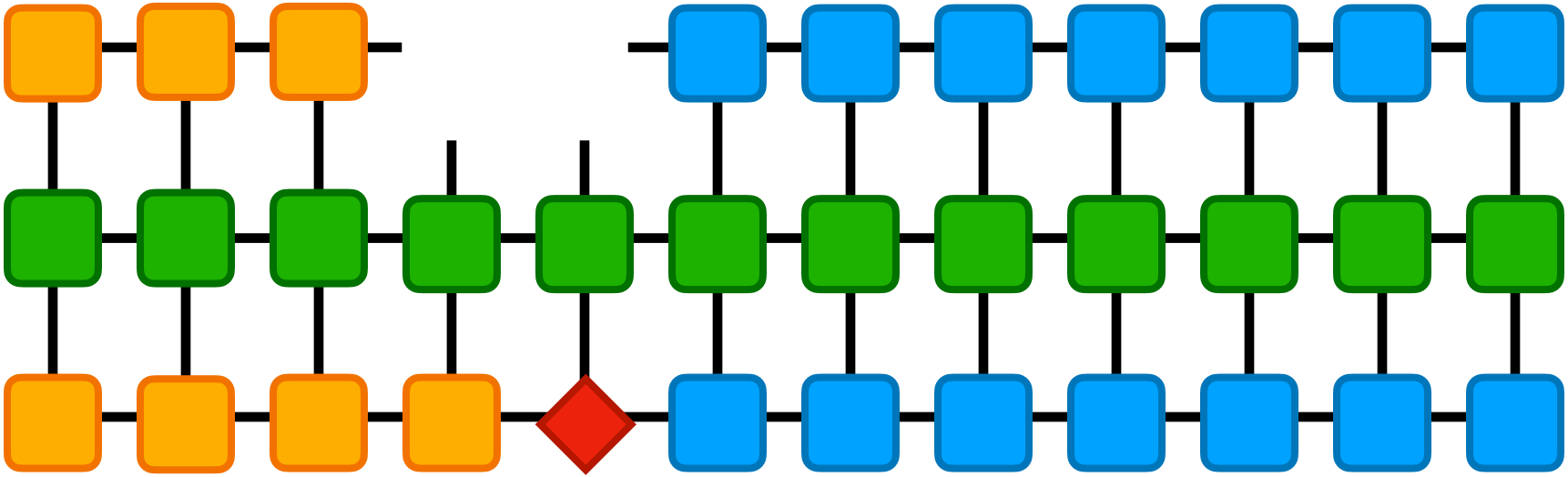

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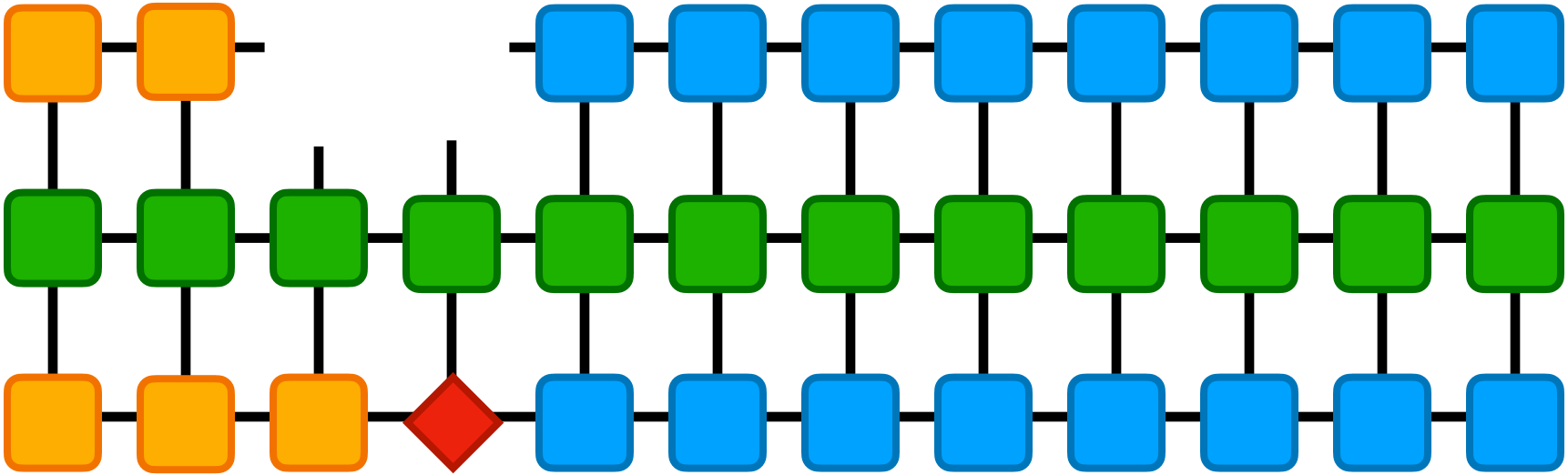

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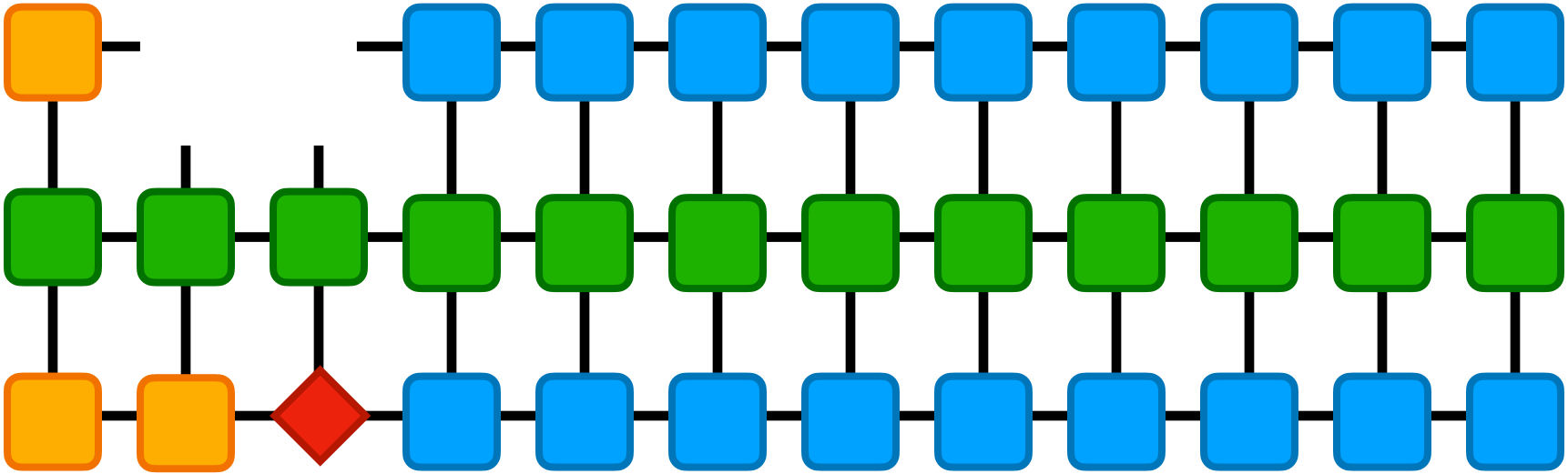

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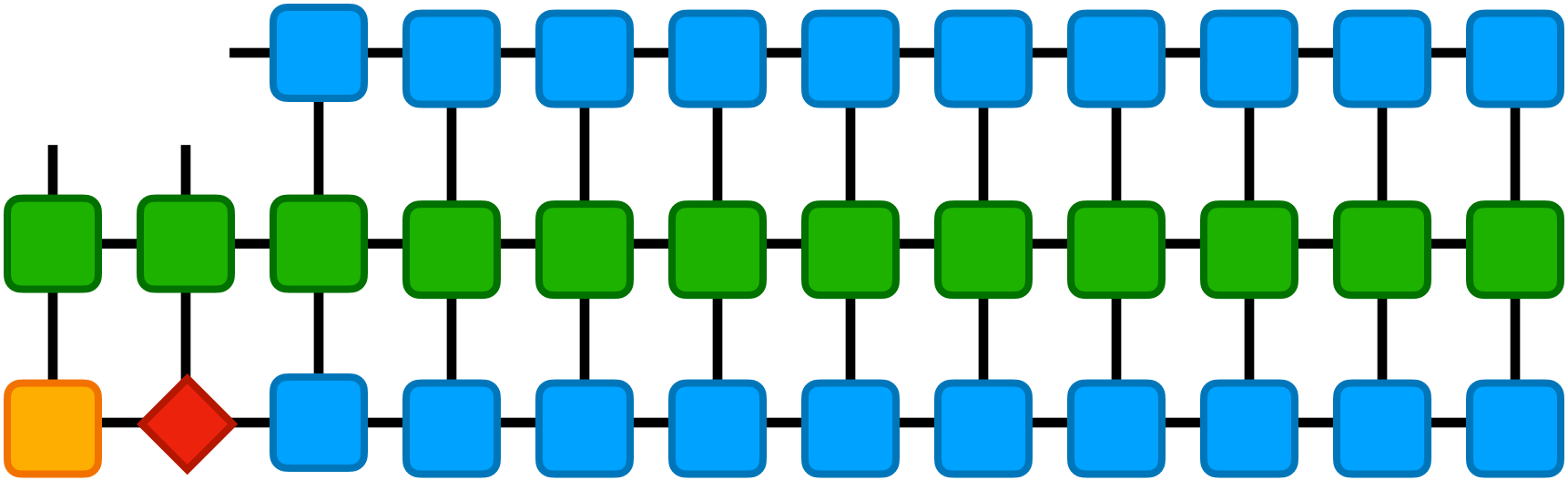

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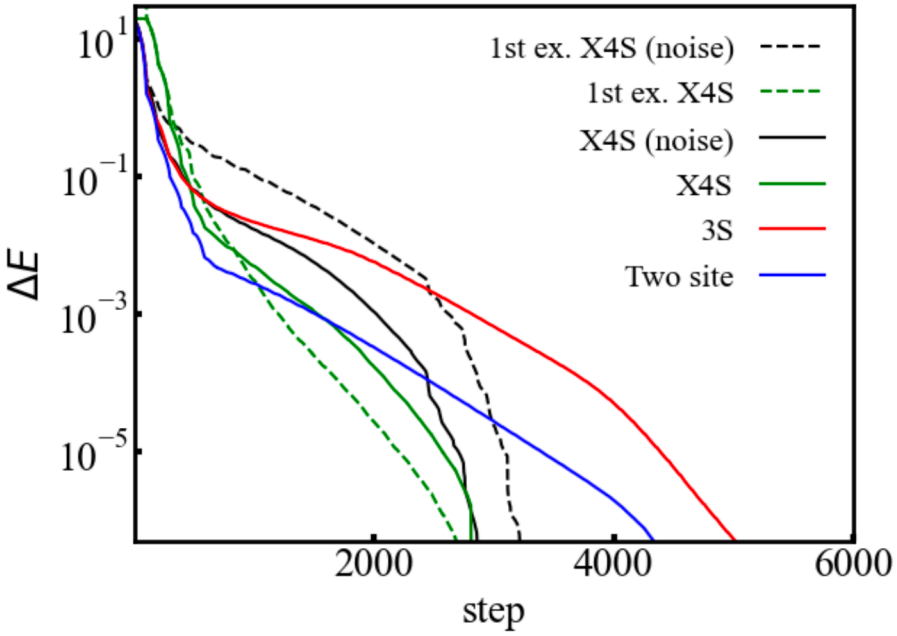
Efficient description of entangled states for excitations



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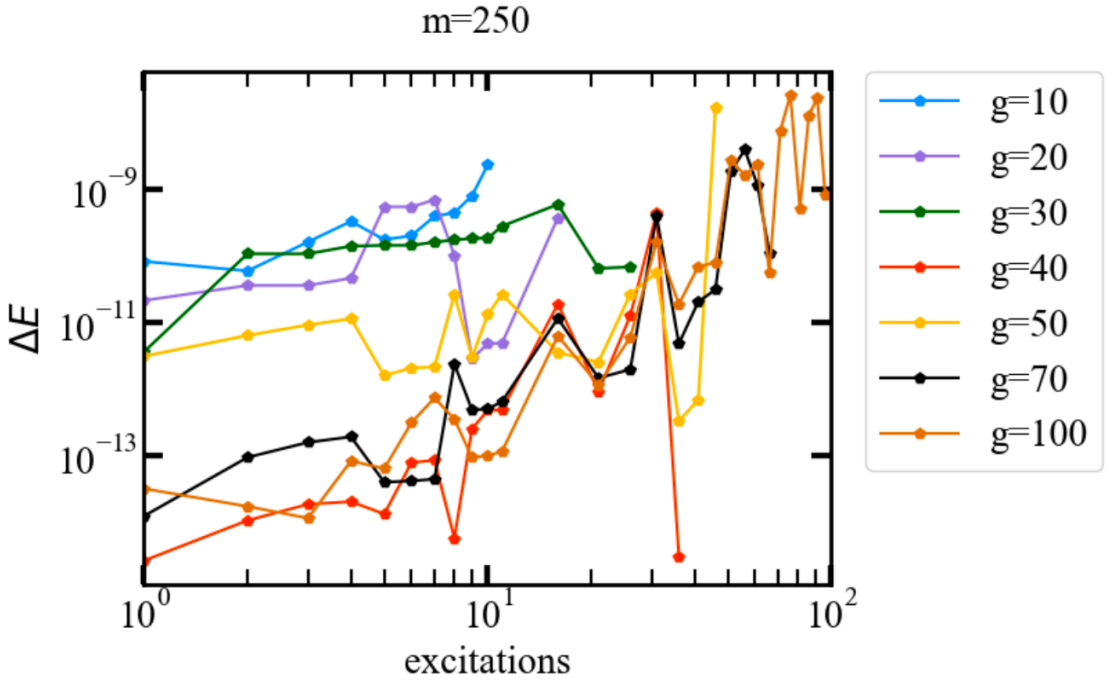
Efficient description of entangled states for excitations



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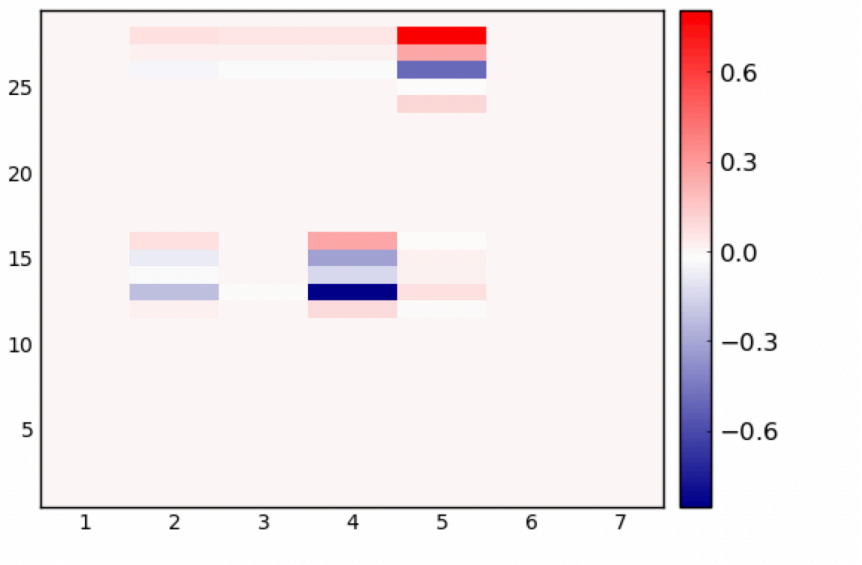

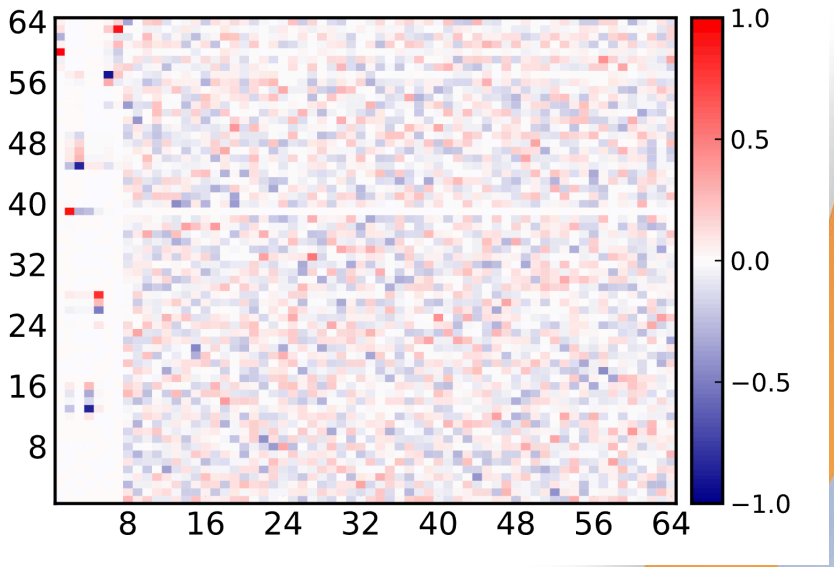

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T.E. Baker, N. Seif, *coming soon*

Conclusion

DMRjulia

- Bundled density matrices
  - Independent
  - Small energy states are similar
  - Novel truncation properties
- Well suited to
  - Gapless systems
  - Volume law entanglement

Build your own tensor network library:
DMRjulia I. Basic library for the density matrix renormalization group

Thomas E. Baker[1,2] and Martin P. Thompson[2]

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(Dated: September 8, 2021)

An introduction to the density matrix renormalization group is contained here, including coding examples. The focus of this code is on basic operations involved in tensor network computations, and this forms the foundation of the DMRjulia library. Algorithmic complexity, measurements from the matrix product state, convergence to the ground state, and other relevant features are also discussed. The present document covers the implementation of operations for dense tensors into the Julia language. The code can be used as an educational tool to understand how tensor network computations are done in the context of entanglement renormalization or as a template for other codes in low level languages. A comprehensive Supplemental Material is meant to be a "Numerical Recipes" style introduction to the core functions and a simple implementation of them. The code is

021

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TUTORIAL

Méthodes de calcul avec réseaux de tenseurs en physique

Thomas E. Baker, Samuel Desrosiers, Maxime Tremblay et Martin P. Thompson

Résumé : Cet article se veut un survol des réseaux de tenseurs et s'adresse aux débutants en la matière. Nous y mettons l'accent sur les outils nécessaires à l'implémentation concrète d'algorithmes. Quatre opérations de base (remodelage, permutation d'indices, contraction et décomposition) qui sont couramment utilisées dans les algorithmes de réseaux de tenseurs y sont décrites. Y seront aussi couverts la notation diagrammatique, intrication, les états en produit de matrices (MPS), les opérateurs en produit de matrices (MPO), état projeté de paires intriquées (PEPS), l'approche par renormalisation d'enchevêtrement multi-échelle (MERA), la décimation par bloc d'évolution temporelle (TEBD) et le groupe de renormalisation de tenseurs (TRG).

Mots-clés : réseaux de tenseurs, décomposition en valeurs singulières, intrication.

Abstract : This article is an overview of tensor networks and is intended for beginners in this field. We focus on the tools required for the concrete implementation of algorithms. Four basic operations (remodelling, permutation of indices, contraction, and decomposition) commonly used in tensor network algorithms are described. This study also covers diagrammatic notation, entanglement, matrix product states (MPS), matrix product operators (MPO), projected entangled pair state (PEPS), multi-scale entanglement renormalization ansatz (MERA), time evolving block decimation (TEBD), and tensor renormalization group (TRG).

Keywords : tensor networks, singular value decomposition, entanglement.

1. Introduction

Les méthodes exactes de résolution de systèmes quantiques sont difficiles à appliquer aux problèmes de grande taille. Il est alors nécessaire d'utiliser des méthodes approximatives et les réseaux de tenseurs figurent parmi les méthodes les plus utilisées à cet effet. Les méthodes des réseaux de tenseurs se basent

Dans cette revue des réseaux de tenseurs, nous nous concentrons sur les opérations de base nécessaires à la manipulation des tenseurs. À la section 2, nous commençons par une discussion de ce que sont les tenseurs. À la section 3, nous introduisons une notation schématique qui permet de simplifier le traitement analytique des réseaux de tenseurs. À la section 4, nous présentons quatre opérations de base s'appliquant aux tenseurs. Dans la