

Моделирование задач статистической механики методом отжига популяций

Lev Shchur

Landau Institute for Theoretical Physics
and
National Research University Higher School of Economics

Российская Академия Наук

МИЭМ Московский институт электроники и математики НИУ ВШЭ

Outline

1. HPC
2. ECP
3. INCITE
4. TOP500.org and top50.ru
5. Parallel annealing
7. Examples
6. Discussion

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Tarusa, 22-10-2019

Main goal

The big challenge for scientific computing is to develop algorithms and computational frameworks using the parallel architecture efficiently.

There are two approaches:

- Develop a universal framework which potentially is fully scalable;
- Invent an algorithm which is efficient for the particular set of problems.

Examples

There are two approaches:

- *Invent an algorithm which is efficient for the particular set of problems and covers the broad range of problems*

For example, *Population Annealing*

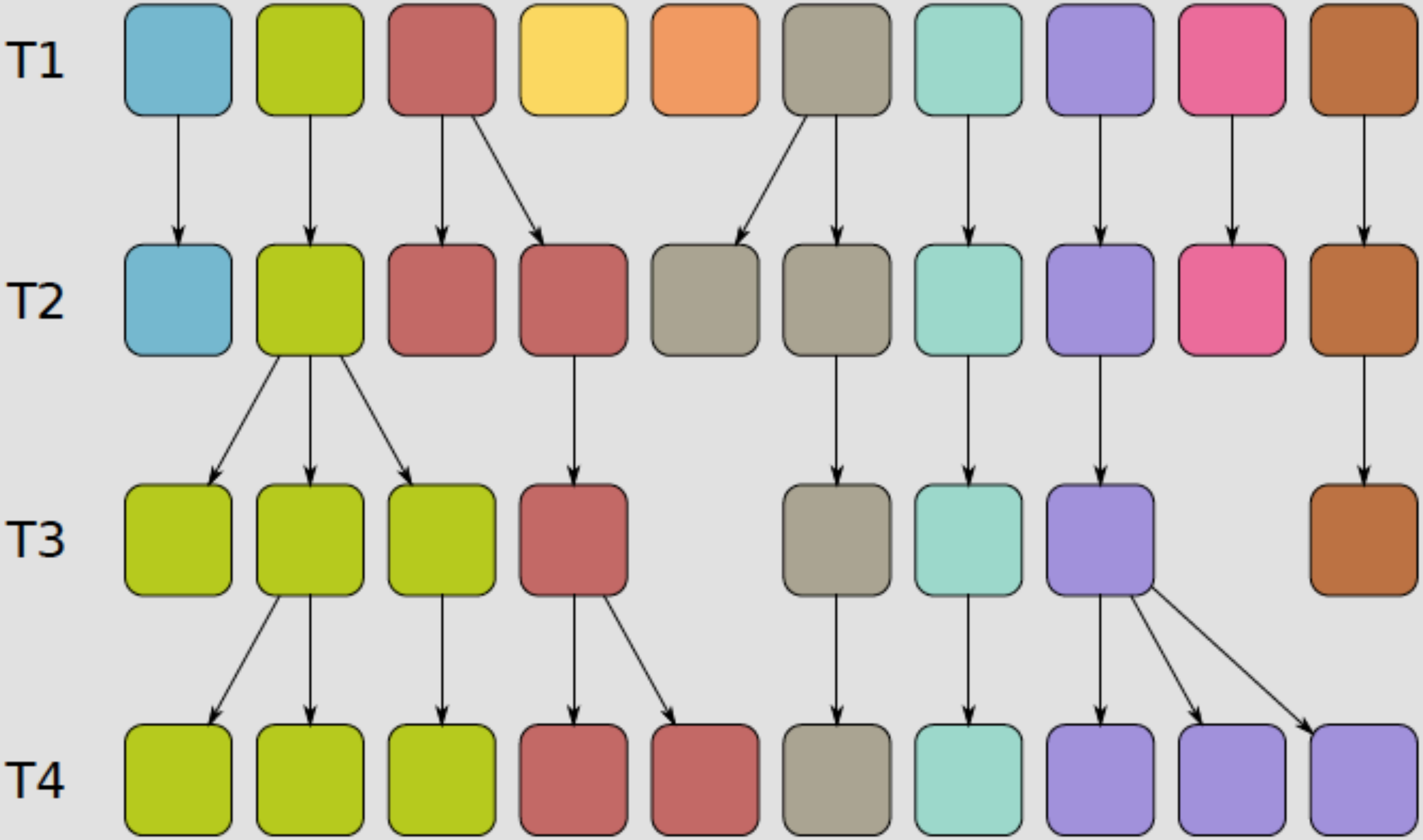
K. Hukushima, Y, Iba, AIP Conf. Proc. 690 (2003) 200

J. Machta, Phys Rev E 82 (2010) 690

Barash, Weigel, Borovsky, Janke, LS, Computer Physics Communications 217 (2017) 341

Can be applied to any system with the partition function

Population annealing



Population Annealing algorithm by Machta

PHYSICAL REVIEW E **82**, 026704 (2010)

Population annealing with weighted averages: A Monte Carlo method for rough free-energy landscapes

J. Machta*

Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA and Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, USA

(Received 4 June 2010; published 18 August 2010)

Population Annealing algorithm by Machta (PAM)

Partition function ratio $Q(\beta_k, \beta_{k-1})$ is given by

$$Q(\beta_k, \beta_{k-1}) = \frac{\sum_{j=1}^{\tilde{R}_{\beta_k}} \exp\left[-(\beta_{k-1} - \beta_k)E_j\right]}{\tilde{R}_{\beta_k}} \quad (1)$$

and normalized weights $\tau_j(\beta_k, \beta_{k-1})$ calculated accordingly by

$$\tau_j(\beta_k, \beta_{k-1}) = \frac{\exp\left[-(\beta_{k-1} - \beta_k)E_j\right]}{Q(\beta_k, \beta_{k-1})} \quad (2)$$

and

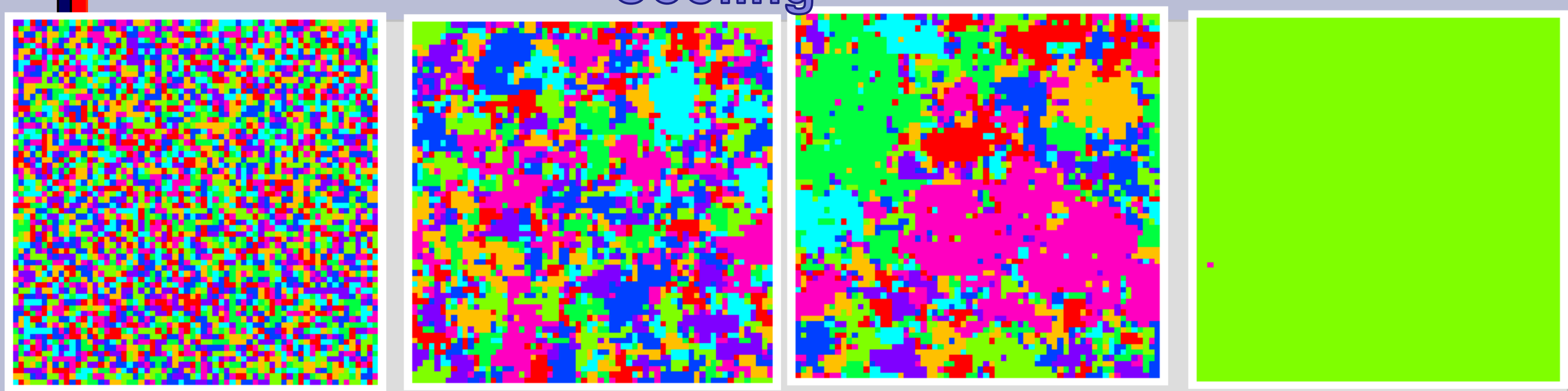
$$\tilde{R}_{\beta_k} = \sum_{j=1}^{\tilde{R}_{\beta_k}} \tau_j(\beta_k, \beta_{k-1}). \quad (3)$$

$$-\beta_k \tilde{F}(\beta_k) = \sum_{i=K}^{k+1} \ln Q(\beta_k, \beta_{k-1}) + \ln \Omega$$

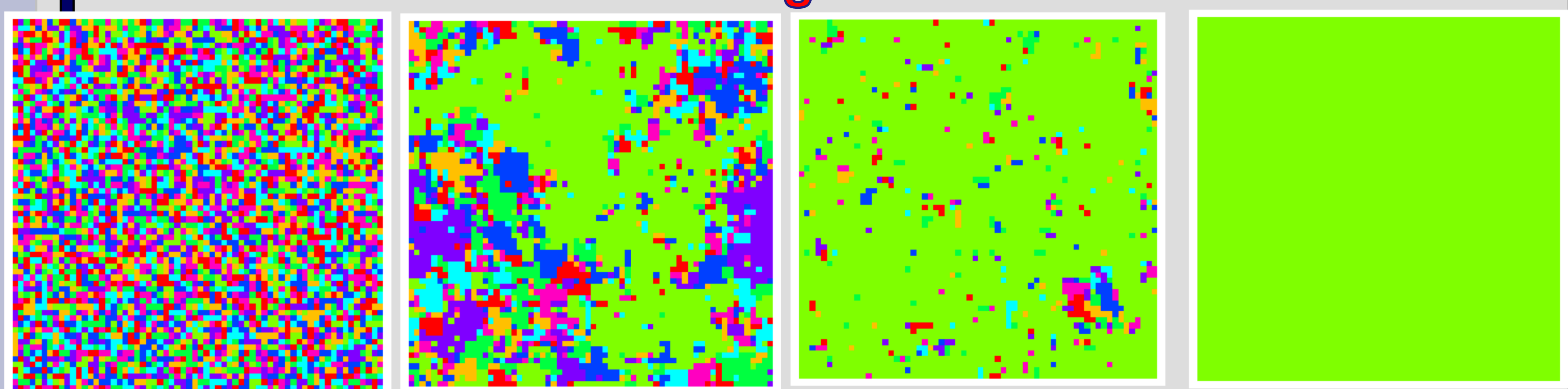
Population Annealing algorithm and 1st order PT

Barash, Janke, Weigel, LS - Eur. Phys. J. Spec. Top. 226 (2017) 595

Cooling

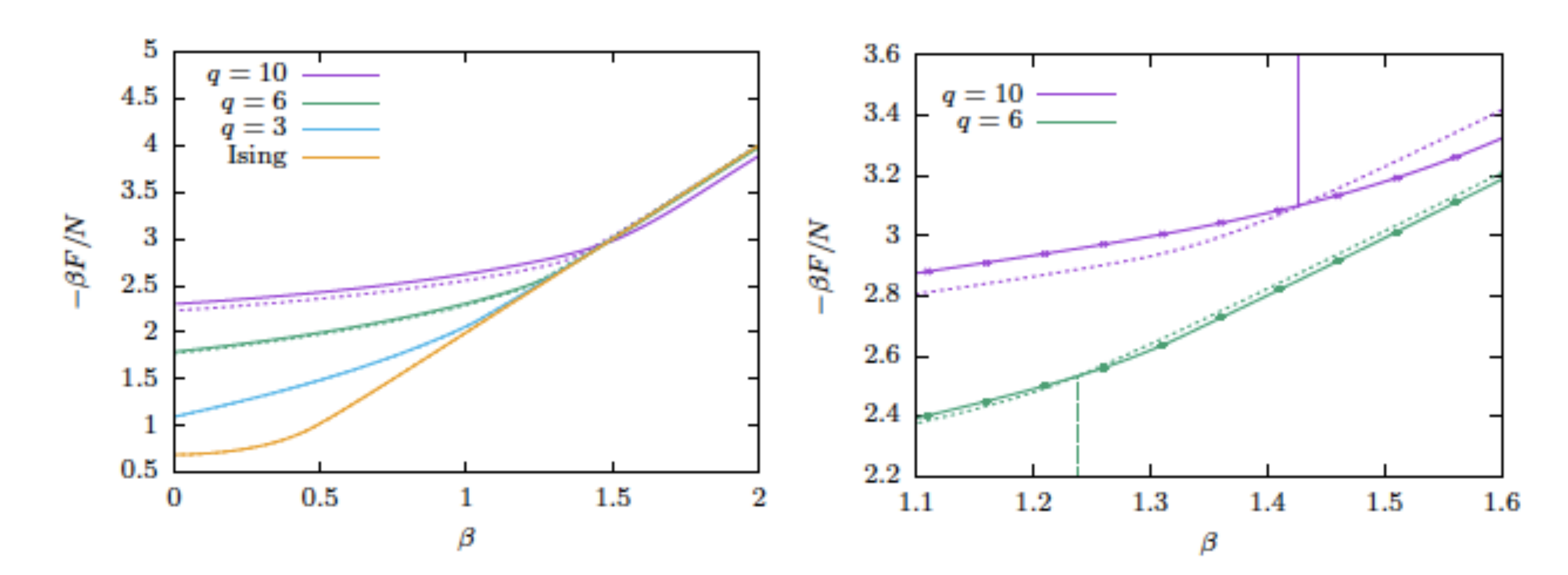


Heating



Population Annealing algorithm and 1st order PT

Barash, Janke, Weigel, LS - Eur. Phys. J. Spec. Top. 226 (2017) 595

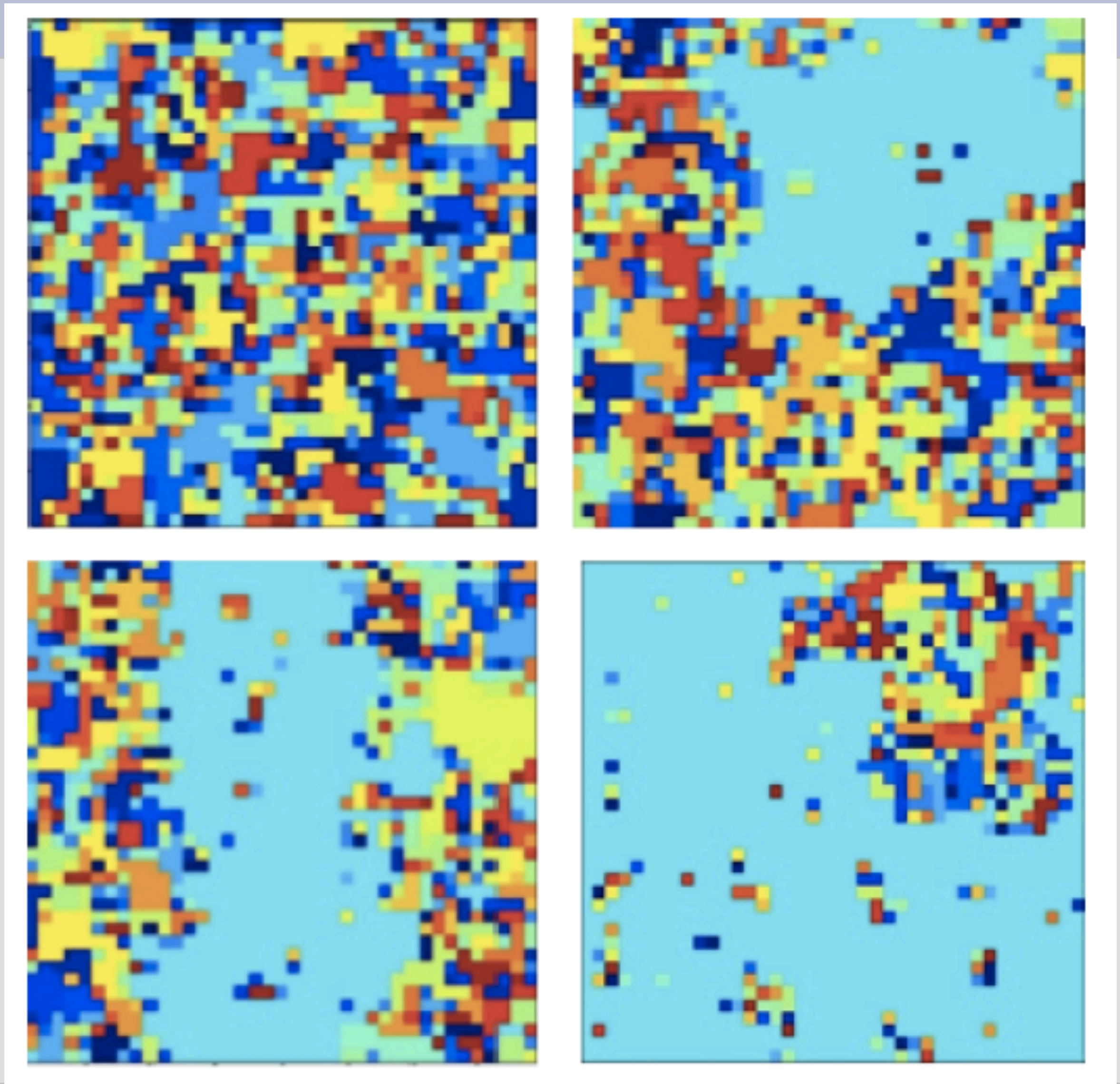


$$\beta_t = \ln(1 + \sqrt{q})$$

$$-\beta_k \tilde{F}(\beta_k) = \sum_{i=K}^{k+1} \ln Q(\beta_k, \beta_{k-1}) + \ln \Omega$$

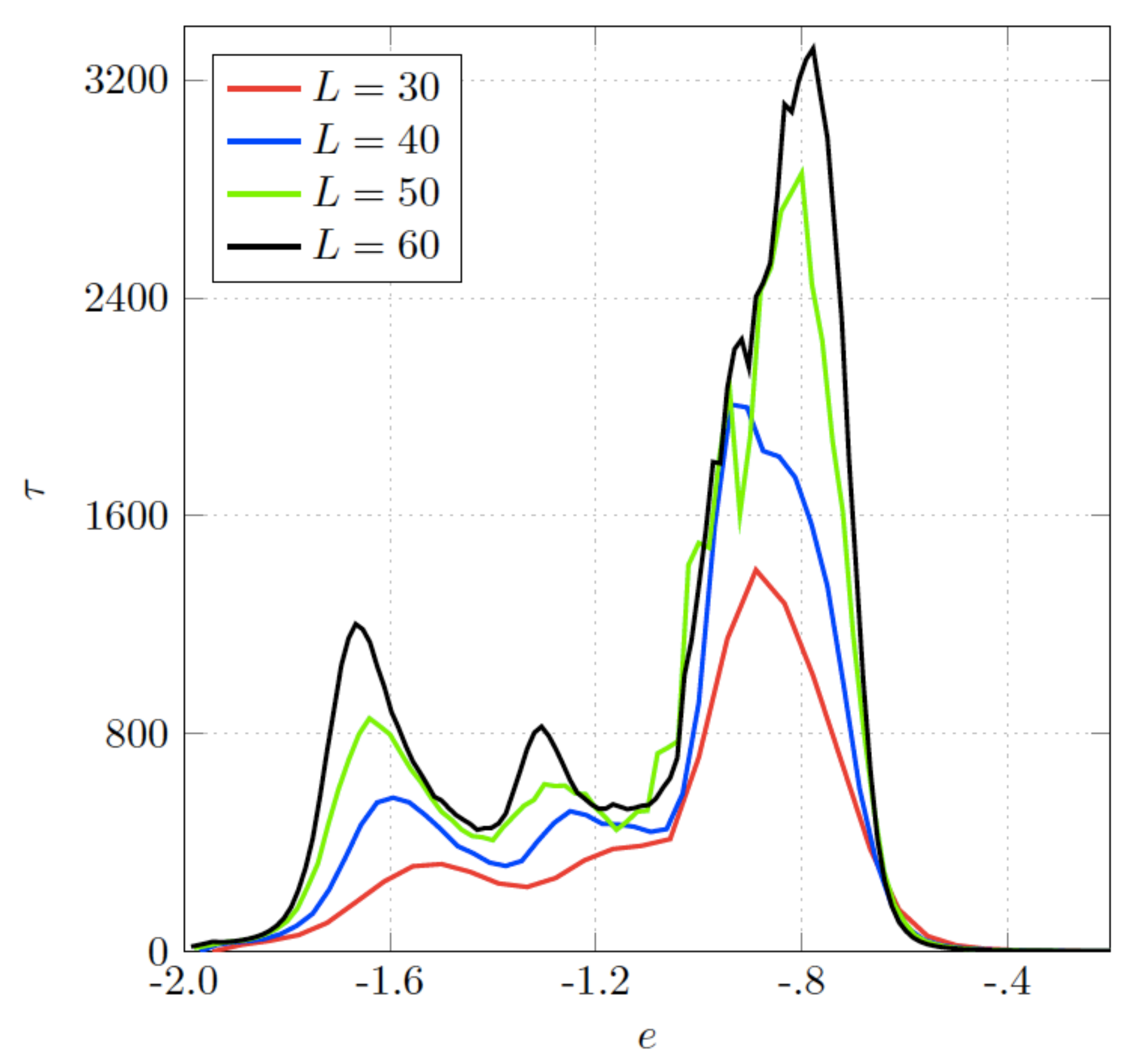
Population Annealing algorithm and 1st order PT

N. Rose and J. Machta – preprint arXiv:1907.07067



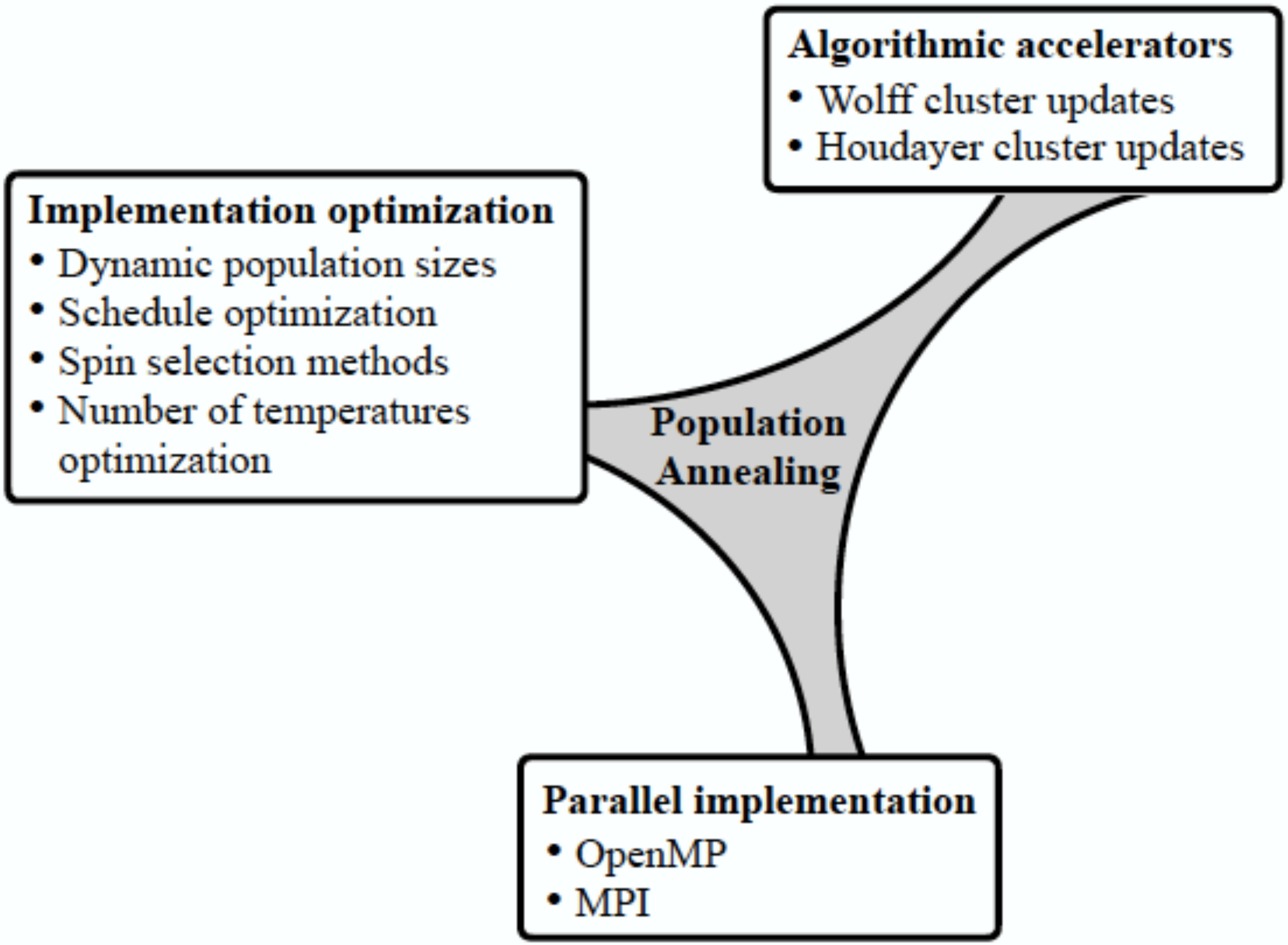
Population Annealing algorithm and 1st order PT

N. Rose and J. Machta – preprint arXiv:1907.07067



Population Annealing algorithm and 1st order PT

Barzegar, Pattison, Wang, Katzgraber, PRE 98, 053308, 2018



Population Annealing algorithm and 1st order PT

Barzegar, Pattison, Wang, Katzgraber, PRE 98, 053308, 2018

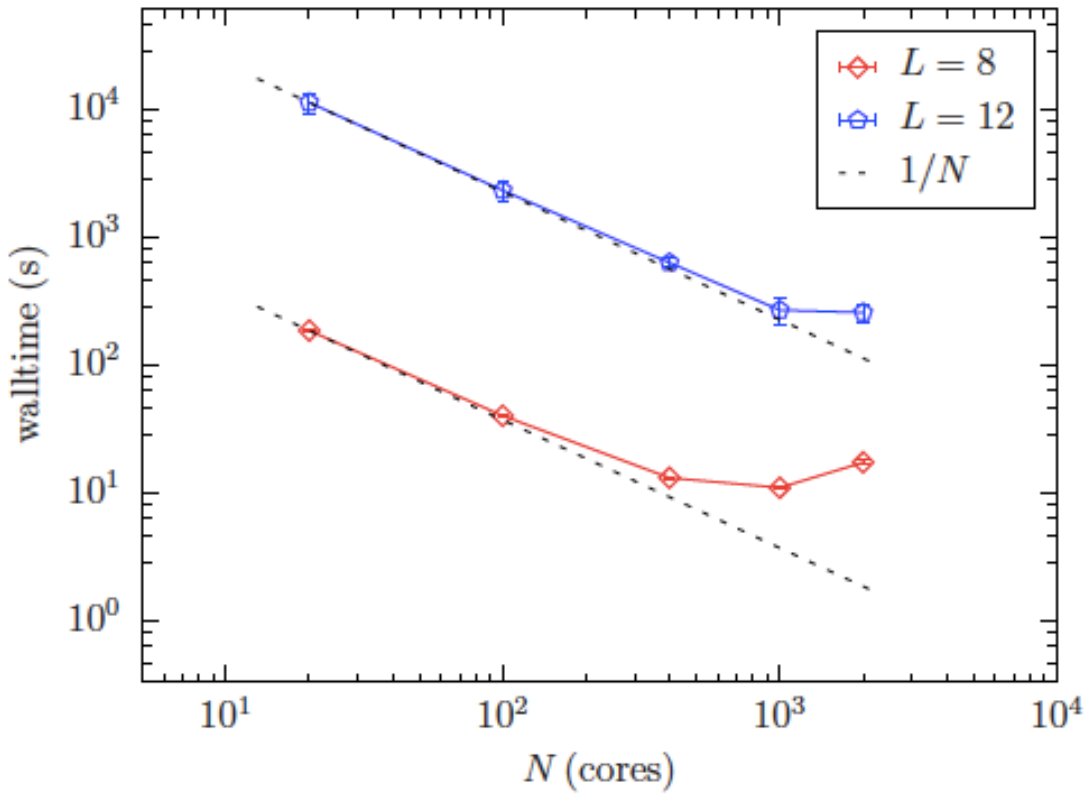


FIG. 10: Scaling of the total wall time as a function of the number of processors N for two system sizes $L = 8$ and $L = 12$. Launching and initialization time are not included. Note that the efficiency becomes better for larger and harder problems. For $L = 12$, the scaling remains $1/N$ up to about 1000 processors. The efficiency then decreases when the time for collecting observables becomes dominant. Note that resampling still takes a relatively small time.

Population Annealing algorithm and 1st order PT

Barash, Weigel, Borovsky, Janke, LS - CPC. 220 (2017) 341

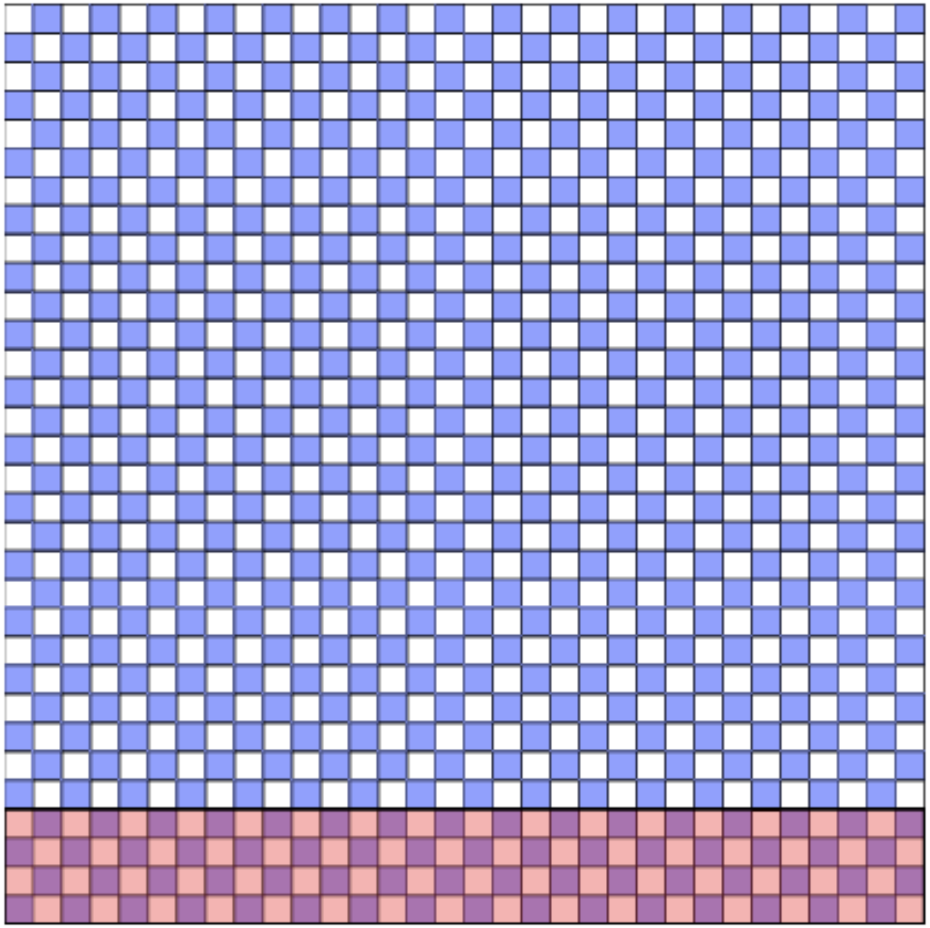


Fig. 1. Diagrammatic representation of the mapping of thread blocks to spins in the updating kernel. The code works with thread blocks of size `EQthreads`. Each block works on a single replica of the population, using its threads to update tiles of size $2 \times$ `EQthreads` spins. To this end, it flips spins on one checkerboard sub-lattice first, moving the tiles over the lattice until it is covered, synchronizes and then updates the other sub-lattice.

Population Annealing algorithm and 1st order PT

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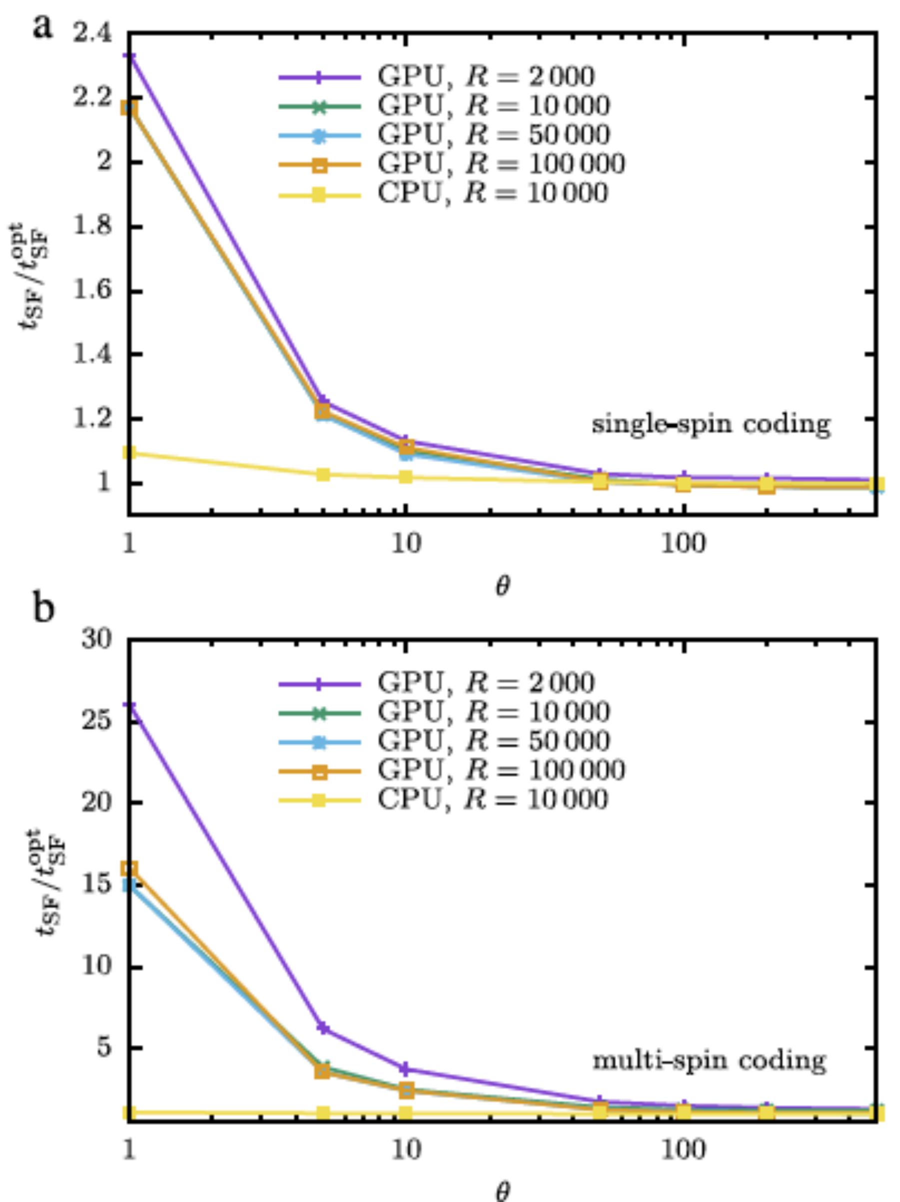

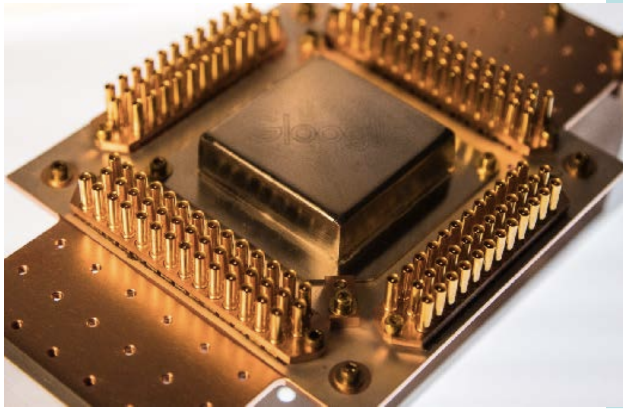

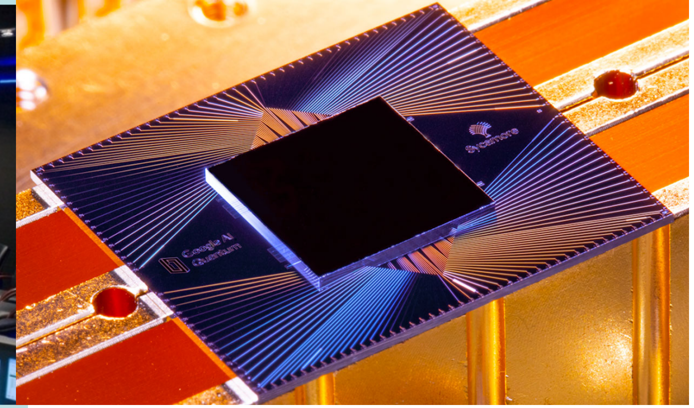

1. **HPC in crisis**
2. **Emergence of HPC facilities-as-service**
3. **Emergence of Big Data development**
4. **Quantum devices and synergy with HPC**
5. **New algorithms and approaches are necessary to keep scientific HPC alive**

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