Efficient space virtualisation for Hoshen–Kopelman algorithm

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In this paper the efficient space virtualisation for the Hoshen–Kopelman algorithm is presented. We observe minimal parallel overhead during computations, due to negligible communication costs. The proposed algorithm is applied for computation of random-site percolation thresholds for four dimensional simple cubic lattice with sites’ neighbourhoods containing next-next-nearest neighbours (3NN). The obtained percolation thresholds are

\[ p_{C}(\text{NN}) = 0.19680(23), \]

\[ p_{C}(\text{2NN}) = 0.08410(23), \]

\[ p_{C}(\text{3NN}) = 0.04540(23), \]

\[ p_{C}(\text{2NN+NN}) = 0.06180(23), \]

\[ p_{C}(\text{3NN+2NN}) = 0.04000(23), \]

\[ p_{C}(\text{3NN+2NN+NN}) = 0.03190(23), \]

where 2NN and NN stand for next-nearest neighbours and nearest neighbours, respectively.

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I. INTRODUCTION

Percolating systems [1–5] are examples of system where purely geometrical phase transition may be observed (see Ref. [6] for recent review). The majority of percolating systems which may be mapped to real-world problems deal with two- or three-dimensional space and ranges from condensed matter physics [7] via rheology [8] and forest fires [9] to immunology [10] and quantum mechanics [11]. However, computer simulations are conducted also for systems with non-physical dimensions \(d\) (up to \(d = 13\)) [12–17].

In classical approach only the nearest neighbours (NN) of sites in \(d\)-dimensional system are considered. However, complex neighbourhoods may have both, theoretical [18, 19] and practical [20–25] applications. These complex neighbourhoods may include not only NN but also next-nearest neighbours (2NN) and next-next-nearest neighbours (3NN).

One of the most crucial feature describing percolating systems is a percolation threshold \(p_{C}\). In principle, this value separates two phases in the system;

- if sites are occupied with probability \(p < p_{C}\) the system behaves as ‘an insulator’,
- while for \(p > p_{C}\) the system exhibit attributes of ‘a conductor’.

Namely, for \(p = p_{C}\) the giant component containing most of occupied sites appear for the first time. The cluster of occupied sites spans from the one edge of the system to the other one (both being \((d-1)\)-dimensional hyper-planes). This allows for direct flow of material (or current) from one to the other edge of the systems. For \(p > p_{C}\) this flow is even easier while for \(p < p_{C}\) the gaps of unoccupied (empty) sites successfully prevent such flow [26].

Among so far investigated systems also four dimensional systems were considered [13–17]. The examples of percolation thresholds for four dimensional lattices and NN neighbours are presented in Tab. I.

TABLE I: The critical values of \(p_{C}\) for various four dimensional lattices with NN neighbours and various site coordination number \(z\).

| lattice        | \(z\) | \(p_{C}\)            | Ref. |
|----------------|------|----------------------|-----|
| diamond        | 5    | 0.2978(2)            | [16]|
| SC             | 8    | 0.196901(5)          | [15]|
| SC             | 8    | 0.196889(3)          | [13]|
| SC             | 8    | 0.1968861(14)        | [14]|
| Kagomé         | 8    | 0.2715(3)            | [17]|
| BCC            | 16   | 0.1037(3)            | [16]|
| FCC            | 24   | 0.0842(3)            | [16]|

In this paper we

- propose an efficient space virtualisation for Hoshen–Kopelman algorithm [27] employed for occupied sites clusters labelling,

- estimate the percolation thresholds for a four dimensional simple cubic (SC) lattice with complex neighbourhoods, i.e. neighbourhoods containing various combinations of NN, 2NN and 3NN neighbours.

While the Hoshen–Kopelman method is good for many problems—for instance, the parallel version of the Hoshen–Kopelman algorithm has been successfully applied for lattice-Boltzmann simulations [28]—probably it is not the best method available to find the thresholds. One can even grow single clusters by a Leath type of
algorithm [29], and find the threshold where the size distribution is power-law, as has been done in many works in three dimensions. For high-dimensional percolation, both Grassberger [14], and Mertens and Moore [30] use a method where you do not even have a lattice, but make a list of the coordinates of all the sites that have been visited, and using computer-science type of structures (linked lists and trees, etc.) one can search if a site has already been visited in a short amount of time. Mertens and Moore [31] have also recently proposed an intriguing method where they use basically invasion percolation (along with the various lists) to grow large clusters that self-organize to the critical point. Both groups have gone up to 13 dimensions using these methods.

II. METHODOLOGY

To evaluate the percolation thresholds the finite-size scaling technique [32–35] has been applied. According to this theory the quantity $X(p)$ characterising the system in the vicinity of critical point $p_C$ scales with the system linear size $L$ as

$$X(p; L) = L^{-x} \cdot F \left( \left( p - p_C \right) L^{1/\nu} \right),$$

(1)

where $F(\cdot)$ is a scaling function, $x$ is a scaling exponent and $\nu$ is a critical exponent associated with the correlation length [2].

For $p = p_C$ the value of $L^x X(p; L) = F(0)$ does not depend on the system linear size $L$ which allows for predicting the position of percolation threshold $p_C$ as curves $L^x X(p; L)$ plotted for various values of $L$ cross each other at $p = p_C$. Moreover, for appropriate selection also the value of critical exponent $\nu$ the dependencies $L^x X(p; L)$ vs. $(p - p_C) L^{1/\nu}$ collapse into a single curve independently on $L$.

Such technique encounters however one serious problem. Namely, numerically deduced curves $L^x X(p; L)$ for various $L$ rather seldom cross each other in a single point, particularly when the number of independent simulations is not huge (see Fig. 1, where examples of dependencies $L^x X(p; L)$ for $L = 20, 40, 80$ and $R = 10^2$ (symbols) and $R = 10^4$ (lines) are presented).

The remedy for this troubles has been proposed by Bastas et al. [36, 37] and even simplified in Ref. [38]. The methodology proposed in Ref. [38] allows for estimation of percolation threshold $p_C$ also for relatively low sampling if the quantity $X(p; L)$ is chosen smartly. Namely, as $X(p; L)$ should be chosen quantity for which scaling exponent $x$ is equal to zero. One of such quantity is the wrapping probability

$$W(p; L) = N(p; L) / R$$

(2)

describing fraction of percolating lattices among $R$ lattices constructed for $p L^d$ occupied sites and fixed values of $p$ and $L$, where $d$ is a geometrical space dimension and $N(p; L)$ is a number of percolating lattices.

According to Refs. [36–38] instead of searching common crossing point of $L^x X(p; L)$ curves for various $L$ one may wish to minimise

$$\lambda(p) \equiv \sum_{i \neq j} \left| H(p; L_i) - H(p; L_j) \right|^2,$$

(3)

where

$$H(p; L) \equiv W(p; L) + 1/W(p; L).$$

(4)

The minimum of $\lambda(p)$ near ‘crossing points’ of $W(p; L)$ curves plotted for various sizes $L$ yields the estimation of percolation threshold $p_C$.

Such strategy allowed for estimation of percolation thresholds $p_C$ for simple cubic lattice ($d = 3$) with complex neighbourhoods (i.e. containing up to next-next-nearest neighbours) with relatively low-sampling ($R = 10^4$) [38]. Unfortunately, reaching similar accuracy as in Ref. [38] for similar linear sizes of the system and for increased space dimension ($d = 4$) requires increasing sampling by one order of magnitude (to $R = 10^5$). This however makes the computations times extremely long. In order to overcome this trouble we propose efficient way of problem parallelisation.

III. COMPUTATIONS

Several numerical techniques allow for clusters of connected sites identification [27, 29, 39, 40]. Here we apply the Hoshen–Kopelman algorithm [27], which allows for sites labelling in a such way, that occupied sites in the same cluster have assigned the same labels and different clusters have different labels associated with them.

The simulations were carried out on Prometheus [41], an Academic Computer Centre Cyfronet AGH-UST operated parallel supercomputer, based on Hewlett-Packard Apollo 8000 Gen9 technology. It consists of 5200 computing 2232 nodes, each with dual 12-core Xeon E5-2680v3 CPUs, interconnected by Infiniband FDR network and over 270 TB of storage space. It supports a wide range of parallel computing tools and applications, including MVAPICH2 [42] MPI implementation for C and Fortran compilers and provides 2.4 PFlops of computing performance, giving it 77th position on November 2017 edition of Supercomputer Top500 list [43].

A. Implementation

One of the problems encountered is high memory size complexity of $O(L^d)$, resulting from space being a hypercube growing in each direction. The memory limit on the machines the program was run did not allow $L \geq 120$. Several solutions were put in consideration, one of which was splitting single simulations’ calculations between nodes. In the classical version of the algorithm there are sequential dependencies both subsequent 3-$d$
FIG. 1: (Colour online). Wrapping probability $W(p; L)$ vs. occupation probability $p$. The results are averaged over $R = 10^2$ (symbols) or $R = 10^4$ (lines) simulations.

slices perpendicular to the axis of percolation and across any given such slice (see Fig. 2a).

If speed is to be ignored, sequential dependencies could be simply distributed across the domains. Then a domain succeeding another one in any direction (e.g. blue one succeeding red one on Fig. 2b) should be sent information on the class of sites in the area of touch ($L^3$ in size) as well as synchronise aliasing arrays. It could be done slice-wise or domain-wise. Slice-wise approach minimises aliasing desynchronisation while domain-wise concentrates communication.

Work between domains can be parallelised. If any domain finds a percolating cluster, it also percolates in the whole hyper-cube, if not, synchronisation of aliasing and both first and last slice cluster ID lists. It requires either totally rebuilding label array or costly label identity checks.

Because of the aforementioned costs and complications, another approach was chosen. Parallelization was only used to accelerate calculations (see Sec. IV A) while the lack of memory problem was solved using space virtualisation.

1. Message Passing Interface

Message Passing Interface (MPI) [44] is prevailing model of parallel computation on distributed memory systems, including dedicated massively parallel processing supercomputers and cluster systems. It is constructed as a library interface, to be integrated with computer programs written in Fortran or C languages. The main advantage of MPI is its portability and ease of use. Software vendors are presented with clearly defined set of
FIG. 2: (Colour online). Parallel subdomains 2-d dependencies model: in-domain across slice (thin horizontal arrows), in-domain between slices (thin vertical arrows), inter-domain (bold horizontal arrows).

(a) Clustering over adjacent slices

(b) Virtualisation step

FIG. 3: (Colour online). Hyperspace buffering in virtualisation (2-d model). Total cost: $O(L^4)$, like without buffering.

2. Space virtualisation

Space virtualisation is possible due to the fact there are very limited information that need to be extracted from the hyper-cube, namely: does it contain at least one percolating cluster. However, any percolating cluster is also percolating for a 4-d slice of any depth perpendicular to the percolation axis, including any cut of depth two. Indeed, clusterising any 3-d slice across the percolation axis requires its immediately preceding slice to be fully available as well as clusterised (see Fig. 2a). It implies only three slices are essentially needed for calculations: the current one, the previous one and the first one, represented on Fig. 3a).

Any iteration over slice buffer introduces additional cost of copying the last slice as the next slice’s immediate predecessor. Due to that, minimal buffer of depth three is highly sub-optimal. For any buffer depth $D$, the additional cost of a single iteration over buffer is $O(L^3)$ and $\lfloor L/D \rfloor$ such iterations are needed, for the total cost of buffering being $O(L^4/D)$, which implies $D$ should be as big as possible.

In fact, buffering can even benefit performance in some cases as smaller chunk of memory may be possible to fit in cache along with label aliasing array. If so, the cost of copying can be more than compensated by massive reduction of number of memory accesses.

3. Parallelism

Because calculations are performed sequentially along the percolation axis, sequentially both over a slice and between slices, no asymptotic speed up is gain from that. However, for each state occupation probability $p$, many simulations ($R$) are run for the results to be meaningful, which leads to the total cost of $O(L^4R)$.

As the simulations are fully independent and only their results are to be combined, the program can be speed-up by utilising parallelism over tasks. The only communication needed is collecting the results (whenever a percolating cluster was found or not) at the end of calculations, which is close to $O(1)$. Theoretical cost is then $O(L^4R/N)$, where $N$ is the number of computational nodes.

In practice it is unnecessary to map each task to a separate native process, which would require huge amounts of CPU cores (thousands to hundreds of thousands). However, each simulation has a similar execution time, which means no run-time work re-balancing is needed so MPI processes can be used with tasks distributed equally among them. Optimally, the number of processes should be a divisor of $N$.

Utilising more than one process per node puts additional limit on memory, which implies reduction of vir-
tualisation buffer depth. For $N$ nodes and $C$-core architecture that is:

$$D_2 = D_1/C.$$  \hspace{1cm} (5)

This operation implies additional cost of roughly multiplying buffering costs $C$ times, while reducing all costs $C$ times due to multiplying the total number of tasks, which is a clear advantage. Because of that, every core is assigned a separate process.

Threading could be used within a single node but due to close to no communication between tasks, it would make the code more sophisticated with very little performance advantage (only reducing $O(1)$ cost of communication).

IV. RESULTS

A. Speed-up and efficiency

One of the most frequently used performance metric of parallel processing is speedup [47, 48]. Let $\tau(L^d, 1)$ be the execution time of the sequential algorithm and let $\tau(L^d, N)$ be the execution of the parallel algorithm executed on $N$ processors, where $L^d$ is the size of the computational problem. A speed-up of parallel computation is defined as

$$S(N) = \frac{\tau(L^d, 1)}{\tau(L^d, N)}.$$ \hspace{1cm} (6)

the ratio of the sequential execution time to the parallel execution time. One would like to achieve $S(N) = N$, so called perfect speed-up [49]. In this case the problem size stays fixed but the number of processing elements are increased. This are referred to as strong scaling [48]. In general, it is harder to achieve good strong-scaling at larger process counts since the communication overhead for many/most algorithms increases in proportion to the number of processes used.

Another metric to measure the performance of a parallel algorithm is efficiency, $E$, defined as

$$E(N) = \frac{S(N)}{N}.$$ \hspace{1cm} (7)

Speedup and efficiency are therefore equivalent measures, differing only by the constant factor $N$.

Fig. 4 demonstrates minimal parallel overhead observed during computations, due to negligible communication costs (see Sec. IIIA3).

B. Percolation thresholds

In Fig. 5 we plot wrapping probabilities $W(p; L)$ vs. occupation probability $p$ for various systems sizes $L (40 \leq L \leq 140)$ and various complex neighbourhoods (which contain various neighbours from NN to 3NN+2NN+NN). In the same figure we also present the dependencies $\lambda(p)$ in semi-logarithmic scale. The local minimum of $\lambda(p)$ near the interception of $W(p; L)$ for various $L$ indicates the percolation threshold $p_C$ obtained with Bastas et al. algorithm.

As we can see in Fig. 5 the true value of $p_C$ is hidden in the interval of the length of $2\Delta p$, where $\Delta p = 10^{-4}$ is the scanning step of occupation probability $p$. With believe that true value of $p_C$ is homogeneously distributed in this interval we can estimate the uncertainty of the percolation threshold $u(p_C) = 2\Delta p/\sqrt{3} \approx 0.00023$.

TABLE II: The values of percolation thresholds $p_C$ for SC lattice in four dimensional space ($d = 4$) and for various neighbourhoods as deduced from Fig. 5.

\begin{tabular}{|c|c|c|}
\hline
neighbourhood & $z$ & $p_C$ \\
\hline
NN & 8 & 0.19680(23) \\
2NN & 24 & 0.08410(23) \\
2NN+NN & 32 & 0.06100(23) \\
3NN & 32 & 0.04540(23) \\
3NN+NN & 40 & 0.04000(23) \\
3NN+2NN & 58 & 0.03310(23) \\
3NN+2NN+NN & 64 & 0.03190(23) \\
\hline
\end{tabular}

The estimated values of $p_C$ together with its uncertainties are collected in Tab. II. The table shows also the coordination numbers $z$ of sites for every considered complex neighbourhoods ranging from NN to 3NN+2NN+NN.
FIG. 5: (Colour online). Wrapping probability \( W(p; L) \) (lines, left axis) and the value \( \lambda(p) \) (symbols, right axis) vs. occupation probability \( p \). The results are averaged over \( R = 10^5 \) simulations.

Please note, that system with 2NN neighbours corresponds to 4-d FCC lattice. The obtained threshold \( p_C(2\text{NN}) \approx 0.08410(23) \) agrees within the error bars with earlier estimation \( p_C(\text{FCC}) \approx 0.0843(3) \) mentioned in Tab. I.

V. CONCLUSIONS

In this paper the memory virtualization for the Hoshen–Kopelman [27] is presented. Due to minimal and constant cost of communication between processes the perfect speed-up (\( S(N) \approx N \)) is observed.

The achieved speed-up allows for computation—in reasonable time—the wrapping probabilities \( W(p; L) \) (Eq. (2)) up to linear size of \( L = 140 \) in \( d = 4 \) dimensional space, i.e. for systems containing \( 3.8416 \times 10^8 \) sites realized \( 10^4 \) times.

The finite-size scaling technique (see Eq. (1) and Sec. II) combined with Bastas et al. technique [36–38] allows for estimation of percolation thresholds for simple cubic lattice in \( d = 4 \) and for neighbourhoods ranging from NN to 3NN+2NN+NN with the accuracy \( u(p_C) = 23 \times 10^{-5} \).

The estimated values of \( p_C \) together with its uncertainties are collected in Tab. II. Our results enriches earlier studies regarding percolation thresholds for complex neighbourhoods on square [50] or three-dimensional SC [38, 51] lattices.
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Appendix A: Program description

The program (Listing 1) was written in Fortran 95 [52] and compiled using Intel Fortran compiler ifort. It follows purely procedural paradigm while utilising some array-manipulation features.

The program's parameters are read from command line. All of them are integers and should be simply written one after another, as all of them are mandatory. They are the following:

- \( L \) — linear size of the problem,
- \( p_{\text{min}} \) — minimal occupation probability to be checked,
- \( p_{\text{max}} \) — maximal occupation probability to be checked,
- \( p_{\text{step}} \) — loop step over probabilities range,
- \( N_{\text{run}} \) — number of simulations for each value of \( p \).

All the parameters and dynamically allocated memory is the same through all the program, which loops through over the examined range of probability from \( p_{\text{min}} \) to \( p_{\text{max}} \) with step \( p_{\text{step}} \). For any given \( p \), all processes run subsequent tasks in parallel to each other, only sending results to the main process (through \( \text{MPI\_sum} \)) after finishing all the tasks for the given value of \( p \).

Sites are given labels according to Hoshen–Kopelman algorithm. There are two kinds of special labels: \FILL\_LABEL, having the lowest possible value, and \EMPTY\_LABEL, having the highest one. Each new casual label is given a successively increasing number. Thanks to that, reclassifying requires no filling checking (although aliasing still does) and checking for percolation is a simple comparison of labels after reclassification: any label with value less than the last label of the first slice is percolating (\HAS\_PERCOLATION function).

Hyper-cubic space is virtualised (see Sec. III A) with merged filling and labelling (conditional at l. 173). Then if a new cluster is made (function \IS\_NEW\_CLUSTER), the site is given a label represented by a successive integer number. If not, cluster surrounding the site are merged (subroutine \MERGE\_CLUSTER). At the end of the buffer (l. 202-209), the last line is copied before the starting line and the process starts again until the virtual depth of \( L \). The first slice is additionally stored separately (l. 191-199).

The program contains basic time measurement.

Appendix B: Source files

The program uses main program (Listing 1), makefile (Listing 2) and batch file (Listing 3).

Makefile is a standard single-target building tool. It provides two commands: ‘build’ (or ‘all’) and ‘clean’. Four parameters can be changed:

- \( \text{FC} \) — Fortran compiler to be used,
- \( \text{PAR\_FC} \) — Fortran parallel (MPI) compiler to be used,
- \( \text{RM} \) — cleaning operation,
- \( \text{SRC} \) — source file.

Batch file runs the executable as a new task on cluster. It contains both program’s run-time parameters and task parameters. Task parameters are the following:

- \(-J \ <\text{name}>\) — name of the task,
- \(-N \ <\text{number}>\) — number of nodes to run the task on,
- \(-\text{ntasks\_per\_node}=\ <\text{number}>\) — number of tasks per node, optimally the same as the number of cores on the given architecture,
- \(-\text{time}=\ <\text{HH}:\text{MM}:\text{SS}>\) — time limit for the task,
- \(-A \ <\text{grant}>\) — name of the computational grant,
- \(-\text{output}=\ <\text{file}>\) — file to which the output will be redirected,
- \(-\text{error}=\ <\text{file}>\) — file to which the error information will be redirected.

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The terminology of material flow between edges of the system comes from the original papers introducing the percolation term [1] in the subject of rheology.
Listing 1: Fortan95 code allowing for direct reproduction of the results presented in Figs. 1 and 5.

```fortran
program pi_4d_2n3n4n
  use ifport, only: rand
  use mpi
  implicit none

  ! time measurement
  real :: start, finish

  ! random seed
  integer :: seed

  ! loop counters
  integer :: i_main, i, j, k, m, hb
  integer :: irun, N_run, maxlabel

  ! maximum L so that the whole hypercube fits into the buffer,
end program pi_4d_2n3n4n
```
! determines buffer's size as (MAX_L+4)**4
integer, parameter :: MAX_L = 110

! minimum depth of the buffer
! the lower, the flatter it can get (and more copying is involved)
! depth is the first dimension (i) so the copying cost should be minimal
integer, parameter :: MIN_DEPTH = 10

! hypercube's edge's length (and length with reserved space)
! experimental limit is L = 418 (L+4 == 422)
integer :: L, L4

! probability of filling a site
real :: p, p_min, p_max, p_step

! percentage of systems with a percolating cluster
double precision :: perc_local, perc

! label for each site
integer, dimension(:, :, :, :), allocatable :: label

! label reduction (aliasing) table
integer, dimension(:, :), allocatable :: iclass

! label for filled sites, has to be smaller than any other label
integer :: FILL_LABEL

! label for empty sites, has to be greater than any other label
integer :: EMPTY_LABEL

! communication
integer :: world_comm, nproc, rank, root_rank, ierror

! string buffer
character(len=20) :: str_buffer

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! start communication
world_comm = Mpi_Comm_World
call Mpi_Init(ierror)
call Mpi_Comm_Size(world_comm, nproc, ierror)
call Mpi_Comm_Rank(world_comm, rank, ierror)
root_rank = 0

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! start random engine
call system_clock(seed) ! any random seed, basically
call srand(seed)

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! read options
if(rank == root_rank) then
call cpu_time(start)
end if

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! read parameters
if(command_argument_count() < 5) then
if(rank == root_rank) then
print *, 'Toofew_arguments,expected_5:_,L,_,p_min,_,p_max,_,p_step,_,N_run'
end if
call abort
end if
str_buffer = ""
call get_command_argument(1, str_buffer)
read(str_buffer, fmt="(I)") L
str_buffer = ""
call get_command_argument(2, str_buffer)
read(str_buffer, fmt="(F)") p_min
str_buffer = ""
call get_command_argument(3, str_buffer)
read(str_buffer, fmt="(F)") p_max
str_buffer = ""
call get_command_argument(4, str_buffer)
read(str_buffer, fmt="(F)") p_step
str_buffer = ""
call get_command_argument(5, str_buffer)
read(str_buffer, fmt="(I)") N_run

L4 = L**4

if(rank == root_rank) then
  print *, '#/uni24234D:/uni24232N3N4N'
  print *, '#/uni2423/uni2423/uni2423L/uni2423/uni2423/uni2423N_run/uni2423/uni2423/uni2423L4 '
  print *, '#' , L, N_run, L4
end if

allocate(label(depth => space_depth(L+4, L+4, L+4, L+4)))

if(depth /= L+4) then
  ! buffering can even give a minor speedup
  if(depth > MIN_DEPTH) then
    if(rank == root_rank) then
      print *, '#_Big_L_value._Buffering_with_size:_', depth
    end if
    else
      if(rank == root_rank) then
        print *, '#_Too_big_L_value._Abort'
      end if
    call abort
  end if
end if

allocate(label(depth, L+4, L+4, L+4))
allocate(iclass(L4/2+2))
FILL_LABEL = lbound(iclass, 1)
EMPTY_LABEL = ubound(iclass, 1)
end associate

! main calculations part

! all processes share the same probability...
do p = p_min, p_max, p_step

perc_local = 0.0d0

! ...but each process calculates a separate simulation
do irun = rank+1, N_run, nproc
  call initialize(maxlabel, label, iclass)
  ! over the edge with buffer depth as step
  do i_main = 0, L-1, size(label,1)-4
    hb = min(ubound(label,1)-2, L-1 - i_main + lbound(label,1)+2)
    do i = lbound(label,1)+2, hb
      do j = lbound(label,2)+2, ubound(label,2)-2
        do k = lbound(label,3)+2, ubound(label,3)-2
          do m = lbound(label,4)+2, ubound(label,4)-2
            ! labeling clusters
! fill randomly + check whether filled or not == just rand
if(rand() < p) then
  if(is_new_cluster(label, i, j, k, m)) then
    maxlabel = maxlabel + 1
    label(i, j, k, m) = maxlabel
  else
    call merge_clusters(label, i, j, k, m, iclass)
  end if
else
  label(i, j, k, m) = EMPTY_LABEL
end if
else
  label(i, j, k, m) = EMPTY_LABEL
end if
end do
do
  end do
do
  end do
do
  end do
end do
end do
end do
end do
if(i_main < (L+2) - (size(label, 1) - 4)) then
  ! 3D space first in depth
  ! saved in unused last space as it will be used later
  if(i_main == 0) then
    do j = lbound(label, 2) + 2, ubound(label, 2) - 2
      do k = lbound(label, 3) + 2, ubound(label, 3) - 2
        do m = lbound(label, 4) + 2, ubound(label, 4) - 2
          label(ubound(label, 1), j, k, m) = label(lbound(label, 1) + 2, j, k, m)
        end do
      end do
    end do
  end if
  ! wrapping buffer around
  do j = lbound(label, 2) + 2, ubound(label, 2) - 2
    do k = lbound(label, 3) + 2, ubound(label, 3) - 2
      do m = lbound(label, 4) + 2, ubound(label, 4) - 2
        label(lbound(label, 1) + 0, j, k, m) = label(hb-1, j, k, m)
        label(lbound(label, 1) + 1, j, k, m) = label(hb-0, j, k, m)
      end do
    end do
  end do
end if
! checking if a cluster is spanning whole system
! first 3D space in depth is stored in unused buffer’s part
maxlabel = max_source_label(label, ubound(label, 1))
if(has_percolation(label, hb, maxlabel)) then
  perc_local = perc_local + 1.0d0/(1.0d0*N_run)
end if
end do
end do

! get stats from all processes into root process
call Mpi_Reduce(perc_local, perc, 1, Mpi_Double_Precision, Mpi_Sum, &
                       root_rank, world_comm, ierr)

! combine stats
if(rank == root_rank) then
  print'(F10.6,1X,F7.3)', p, perc
end if
end do
!
! deallocate buffer, cluster classes etc.
deallocate(label)
deallocate(iclass)
if(rank == root_rank) then
  call cpu_time(finish)
  print ('(Time=",f10.3,"_seconds.")', finish=start)
end if

! finalize communication
  call Mpi_Finalize(ierr)
contains
! calculate space depth
integer pure function space_depth(N, M, K, L)
  integer, intent(in) :: N, M, K, L
  space_depth = min((MAX_L+4)**4 / (M*K*L) - 4, N)
end function space_depth

! initialize per location to zero
subroutine initialize(maxlabel, label, iclass)
  integer, intent(out) :: maxlabel
  integer, intent(out), dimension(:, :, :, :) :: label
  integer, intent(out), dimension(:) :: iclass
  maxlabel = FILL_LABEL + 1
  label(:,:,:,1) = EMPTY_LABEL
  do i = lbound(iclass, 1), ubound(iclass, 1)
    iclass(i) = i
  end do
end subroutine

! whether the given site makes a new cluster
logical pure function is_new_cluster(label, i, j, k, m)
  integer, intent(in), dimension(:, :, :, :) :: label
  integer, intent(in) :: i, j, k, m
  is_new_cluster = label(i-1,j,k,m) == EMPTY_LABEL .and. &
  label(i,j-1,k,m) == EMPTY_LABEL .and. &
  label(i,j,k-1,m) == EMPTY_LABEL .and. &
  label(i,j,k,m-1) == EMPTY_LABEL .and. &
  label(i-1,j-1,k,m) == EMPTY_LABEL .and. &
  label(i-1,j+1,k,m) == EMPTY_LABEL .and. &
  label(i-1,j,k+1,m) == EMPTY_LABEL .and. &
  label(i-1,j,k,m+1) == EMPTY_LABEL .and. &
  label(i-1,j,k,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m) == EMPTY_LABEL .and. &
  label(i,j,k-1,m) == EMPTY_LABEL .and. &
  label(i,j,k,m) == EMPTY_LABEL .and. &
  label(i,j,k-1,m+1) == EMPTY_LABEL .and. &
  label(i,j,k,m+1) == EMPTY_LABEL .and. &
  label(i,j,k-1,m+1) == EMPTY_LABEL .and. &
  label(i,j,k,m) == EMPTY_LABEL .and. &
  label(i,j,k,m-1) == EMPTY_LABEL .and. &
  label(i,j,k,m+1) == EMPTY_LABEL .and. &
  label(i,j,k-1,m) == EMPTY_LABEL .and. &
  label(i,j,k-1,m-1) == EMPTY_LABEL .and. &
  label(i,j,k+1,m) == EMPTY_LABEL .and. &
  label(i,j-1,k,m) == EMPTY_LABEL .and. &
  label(i,j-1,k,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k,m) == EMPTY_LABEL .and. &
  label(i,j-1,k,m-1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m-1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m-1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
  label(i,j-1,k+1,m+1) == EMPTY_LABEL .and. &
label(i-1,j+1,k,m-1) == EMPTY_LABEL . and . &
label(i-1,j,k,m+1) == EMPTY_LABEL . and . &
label(i-1,j+1,k,m+1) == EMPTY_LABEL . and . &
label(i-1,j-1,k-1,m ) == EMPTY_LABEL . and . &
label(i-1,j+1,k-1,m ) == EMPTY_LABEL . and . &
label(i-1,j-1,k+1,m ) == EMPTY_LABEL . and . &
label(i-1,j+1,k+1,m ) == EMPTY_LABEL .

end function is_new_cluster

! merge clusters connecting at the given point

subroutine merge_clusters(label , i , j , k , m , iclass )
  integer , intent(inout) , dimension(:,:,,:) :: label
  integer , intent(in) :: i , j , k , m
  integer , intent(inout) , dimension(:) :: iclass

  ! reclassifying neighbours

  ! 2N:
  call reclassify(label(i-1,j , k , m ) , iclass )
call reclassify(label(i ,j-1,k , m ) , iclass )
call reclassify(label(i ,j ,k-1,m ) , iclass )
call reclassify(label(i ,j-1,k-1,m ) , iclass )
call reclassify(label( i ,j ,k-1,m+1) , iclass )
call reclassify(label(i ,j ,k ,m-1) , iclass )
call reclassify(label(i ,j+1,k ,m ) , iclass )
call reclassify(label(i ,j-1,k+1,m ) , iclass )
call reclassify(label(i ,j-1,k ,m+1) , iclass )
call reclassify(label(i ,j ,k ,m-1) , iclass )
call reclassify(label(i ,j+1,k ,m-1) , iclass )
call reclassify(label(i ,j ,k-1,m-1) , iclass )
call reclassify(label(i ,j+1,k-1,m ) , iclass )
call reclassify(label( i ,j ,k+1,m ) , iclass )
call reclassify(label(i ,j ,k ,m+1) , iclass )
call reclassify(label(i ,j+1,k ,m+1) , iclass )
call reclassify(label(i ,j ,k-1,m+1) , iclass )
call reclassify(label(i ,j+1,k-1,m+1) , iclass )
call reclassify(label(i ,j-1,k ,m+1) , iclass )
call reclassify(label(i ,j+1,k ,m-1) , iclass )
call reclassify(label(i ,j ,k-1,m-1) , iclass )
call reclassify(label(i ,j-1,k ,m+1) , iclass )
call reclassify(label(i ,j ,k+1,m ) , iclass )
call reclassify(label(i ,j+1,k ,m+1) , iclass )
nend subroutine

! good label according to rule:
! a <= b => iclass(a) <= iclass(b)
label( i , j , k , m ) = min( &
  label(i-1,j , k , m ) , &
call label(i , j , k-1 , m ) , &
call label(i , j , k , m-1) , &
call label(i-1,j-1,k , m ) , &
call label(i-1,j+1,k , m ) &
)
! make the label common as iclass

call make_alias(label, i-1,j,k,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
call make_alias(label, i-1,j+1,k ,m , i,j,k,m)
call make_alias(label, i-1,j ,k+1,m, i,j,k,m)
end subroutine merge_clusters

! get maximal label for the 3D space first in depth

integer pure function max_source_label(label, row)
  integer, intent(in) , dimension(:, :, :) :: label
  integer, intent(in) :: row
integer :: j, k, m

max_source_label = 0

do j = lbound(label,2)+2, ubound(label,2)-2
  do k = lbound(label,3)+2, ubound(label,3)-2
    do m = lbound(label,4)+2, ubound(label,4)-2
      if(label(row, j, k, m) /= EMPTY_LABEL) then
        max_source_label = max(max_source_label, &
            label(row, j, k, m))
      end if
    end do
  end do
end do

! whether there is a percolation or not

logical pure function has_percolation(label, row, maxlabel)
integer, intent(in), dimension(:,:),:,:) :: label
integer, intent(in) :: row, maxlabel
integer :: j, k, m

has_percolation = .false.

do j = lbound(label,2)+2, ubound(label,2)-2
  do k = lbound(label,3)+2, ubound(label,3)-2
    do m = lbound(label,4)+2, ubound(label,4)-2
      if(label(row, j, k, m) <= maxlabel) then
        has_percolation = .true.
        return
      end if
    end do
  end do
end do

end function has_percolation

! reduce site's label's aliasing
!
subroutine reclassify(ix, iclass)
integer, intent(inout) :: ix
integer, intent(in), dimension(:) :: iclass

do while (iclass(ix) /= ix)
  ix = iclass(ix)
end do

end subroutine reclassify

! makes one site's cluster an alias for another one

subroutine make_alias(label, i1, j1, k1, m1, i2, j2, k2, m2)
integer, dimension(:,:),:,:) :: label
integer, intent(in) :: i1,:,j1,:,k1,:,m1, i2,j2,k2,m2

if(label(i1,i1,k1,m1) /= EMPTY_LABEL) then
  iclass(label(i1,i1,k1,m1)) = label(i2,j2,k2,m2)
end if

end subroutine

end program pi_4d_2n3n4n

Listing 2: Makefile

RM=rm
FC=ifort
PAR_FC=mpiifort
FLAGS = -g -O3 -no-prec-div -fp-model fast=2 -xHost -ipo -warn all
SRC=pi_4d_2n3n4n.f90
OBJ=${SRC:. f90=.o}
EXE=${SRC:. f90=.exe}

.PHONY: all
all: build

.PHONY: build
build: $(EXE)

$(EXE): $(OBJ)
$(PAR_FC) $(FLAGS) -o $@ $< -module .

$(OBJ): $(SRC)
$(PAR_FC) $(FLAGS) -c -o $@ $<

.PHONY: clean
clean:
$(RM) -f $(EXE) *.o *.mod

Listing 3: Batch file

#!/bin/bash

#SBATCH --job_name=pi_4d_2n3n4n
#SBATCH --ntasks-per-node=24
#SBATCH --time=1:00:00
#SBATCH --partition=kk4d3nn
#SBATCH --output="pi_4d_2n3n4n.out"
#SBATCH --error="pi_4d_2n3n4n.err"

module add plgrid/tools/impi
export FORT_BUFFERED=yes
mpirun -env I_MPI_FABRICS=shm:dapl -env I_MPI_FABRICS_LIST=dapl -env I_MPI_DAPL_UD=enable -env MPIEXEC_PREFIX_DEFAULT=out ./pi_4d_2n3n4n.exe 80 0.030 0.034 0.0001 10000