C/C++ Implementation of kinetic Monte Carlo

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Programming language: C / C++

useful features of C/C++

- Bit-wise logical operator
  - AND &
  - OR |
  - negate ~
- recursive function calls
- C++ object-oriented programming

topics of interest

- data representation
- random number generator
- periodic boundary conditions

example programs

- process-type-list algorithm:
  C program `simple`
- binary-tree algorithm:
  C++ program `tree`

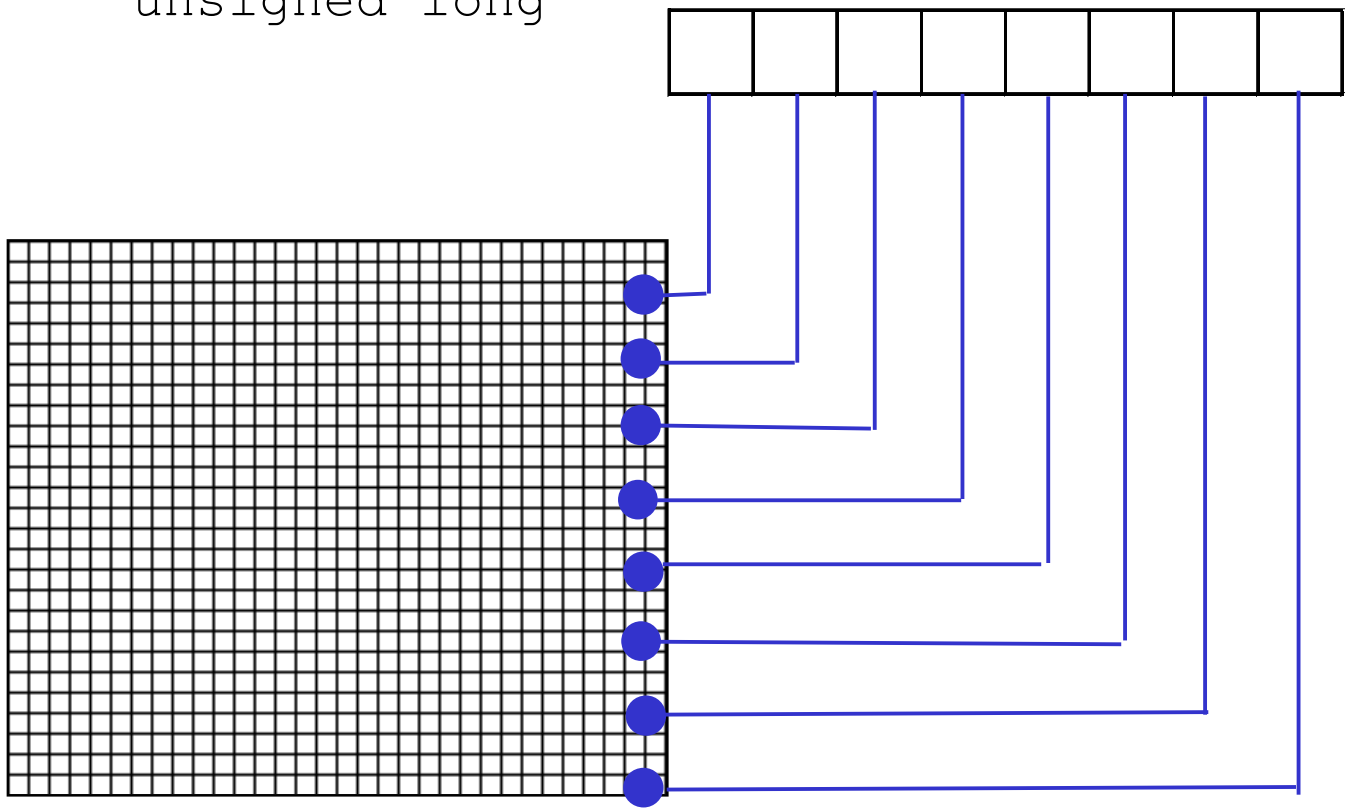
Data representation

- SOS model:
  only 2-dimensional array required to store the local height of the surface
  ```
  int height[i][j]
  ```
- more complex models, e.g with different species:
  3-dimenaional array
  ```
  char lattice[i][j][h]
  #define A_species 0x001
  #define B_species 0x010
  #define C_species 0x100
  ```
  query
  ```
  if (lattice[i][j][h] & A_species) …
  ```
  assignment
  ```
  lattice[i][j][h] |= B_species;
  ```
  removal
  ```
  lattice[i][j][h] &= ~C_species;
  ```

Data representation

- “multispin-coding” in Ising / lattice-gas models

  `unsigned long`



Each bit in a data word addresses one node in a sub-lattice
→ quasi-parallel processing of many spins at a time

Random number generators

- frequently used types of random number generators
  - congruential generators (based on prime cosets spaces)
  - Knuth's subtractive method `irnd`
  - bit-shifting polynomial twisters:
    Mersenne twister `mt19937`
- possible problems
  - repetition period possibly too short
  - single congruential generators have short-time correlations
    solution: interleaved congruetial generators
  - real numbers from congruential generators: trailing digits are "less random" than leading digits
    solution: don't use congruential generators if rate constants differ by orders of magnitude
  - risk of a "blind spot" in the random sequence, processes with very small rates are "overlooked"
    solution: "index-shuffling" in the rate list

Periodic boundary conditions

- modulo operations: possible, but slow
- indirect addressing

```
height[i-1][j] → height[BACK[i]][j]

makePBCs()
{ for (j=1; j<L, j++) BACK[j]= (j-1+L)%L;
  return;}
```

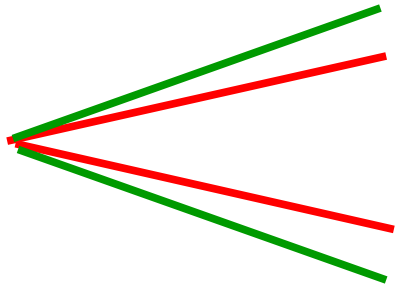
- use powers of 2 for the lattice dimensions, bit mask in address space

```
L= pow(LBL,2);
LL = L-1;
height[i-1][j] → height[(i-1) & LL]][j]
```

Object orientation

```
class Node{
 public:
  Node(char d, char i, char j);
  int select(double rate, char* i, char* j);
  void set_rate(double input_rate);
  double update(void);
  double get_rate(void);
  ~Node();

 protected:
  char depth, ix, jy;
  Node *westnode, *eastnode, *southnode, *northnode;
  double rate;
};
```



Recursive instancies of Node are used to build up the tree of total depth LBL.