"Numerical Precision and the Errors you May not be Aware Of"

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USC | Center for Advanced Research Computing

Enabling scientific breakthroughs at scale

WHAT IS A NUMBER?

- Real
- Imaginary
- Complex
- Integer
- Countable
- Random
- Finite/Infinite
- Positive/Negative
- Rational/Irrational/Transcendental
- Binary/Decimal/Octal/Hexadecimal
- Exact/Approximate
- Floating point

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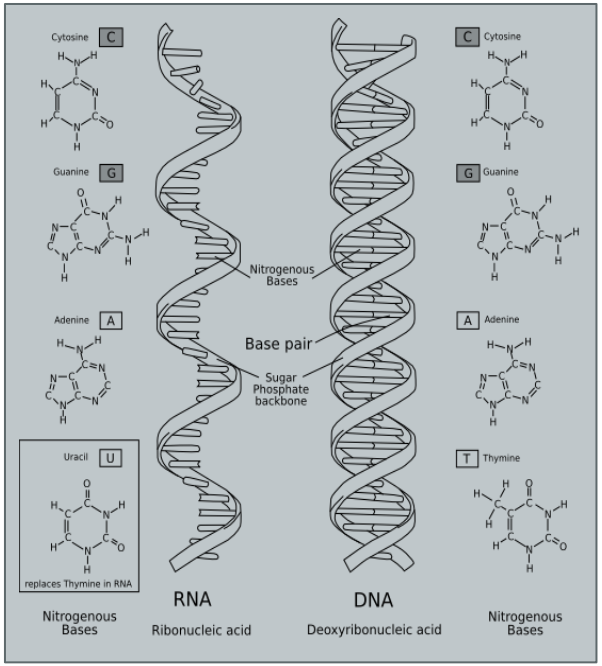
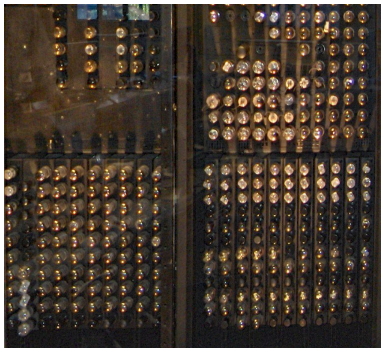
WHAT IS A NUMBER? Storage and Representation



https://en.wikipedia.org/wiki/Data_storage

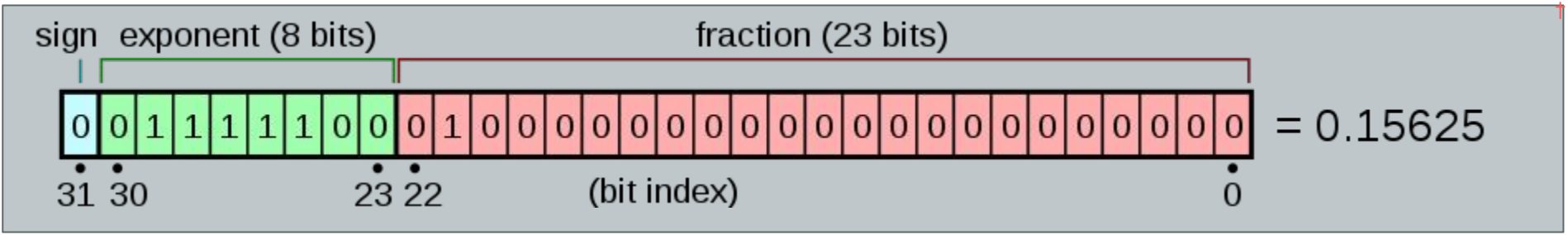


0x0	0	0	1	1	0	0	0	0
0x1	0	0	0	0	0	0	0	0
0x2	0	0	0	0	0	1	0	0
0x3	0	0	0	0	0	0	0	0
0x4	0	0	1	0	0	0	0	0
0x5	0	0	0	0	0	0	0	0
0x6	0	0	0	0	0	0	0	0
0x7	0	0	0	0	0	0	0	0
0x8	0	0	0	1	0	0	0	0
0x9	0	0	0	0	0	0	0	0
0xA	0	0	1	0	0	0	0	0
0xB	0	0	0	1	0	0	0	0
0xC	0	1	0	0	0	0	0	0
0xD	0	0	0	0	1	0	0	0
0xE	0	0	0	1	0	1	0	0
0xF	0	1	0	0	0	1	0	0

WHAT IS A NUMBER? Storage and Representation

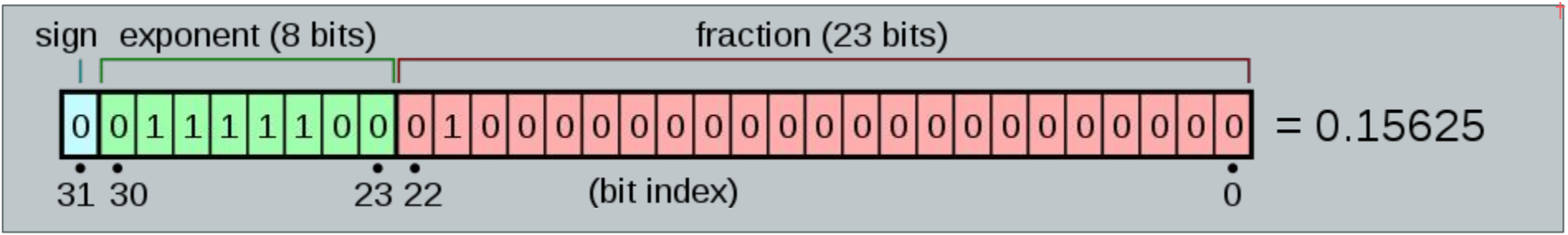
0x0	0	0	1	1	0	0	0	0
0x1	0	0	0	0	0	0	0	0
0x2	0	0	0	0	0	1	0	0
	0	0	0	0	0	0	0	0
	0	0	1	0	0	0	0	0
	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0
0x8	0	0	0	1	0	0	0	0
0x9	0	0	0	0	0	0	0	0
0xA	0	0	1	0	0	0	0	0
0xB	0	0	0	1	0	0	0	0
0xC	0	1	0	0	0	0	0	0
0xD	0	0	0	0	1	0	0	0
0xE	0	0	0	1	0	1	0	0
0xF	0	1	0	0	0	1	0	0

WHAT IS A NUMBER? Machine representation of a floating point number



†https://en.wikipedia.org/wiki/Single-precision_floating-point_format

WHAT IS A NUMBER? Machine representation of a floating point number



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= 1

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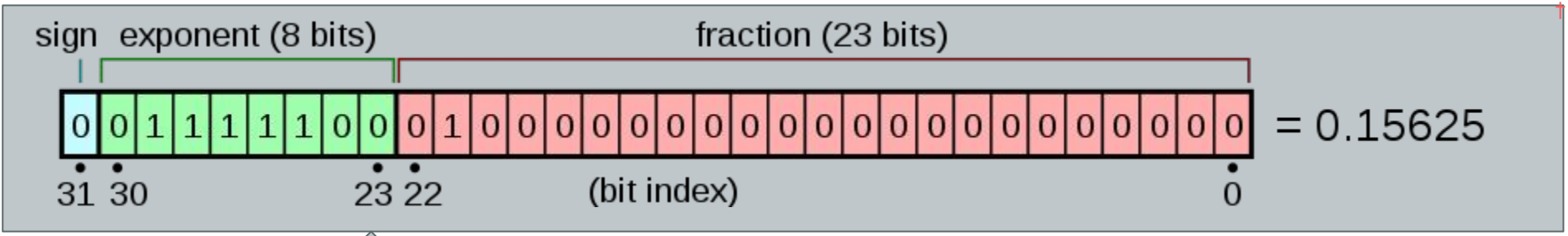

-1^{sign} = **1**

The exponent is 'offset binary' format with a shift of -127, i.e. the exponent is (0*128) + (1*64) + (1*32) + (1*16) + (1*8) + (1*4) + (0*2) + (0*1) **- 127**, or **-3**. This means a factor of $\mathbf{2^{-3}}$.

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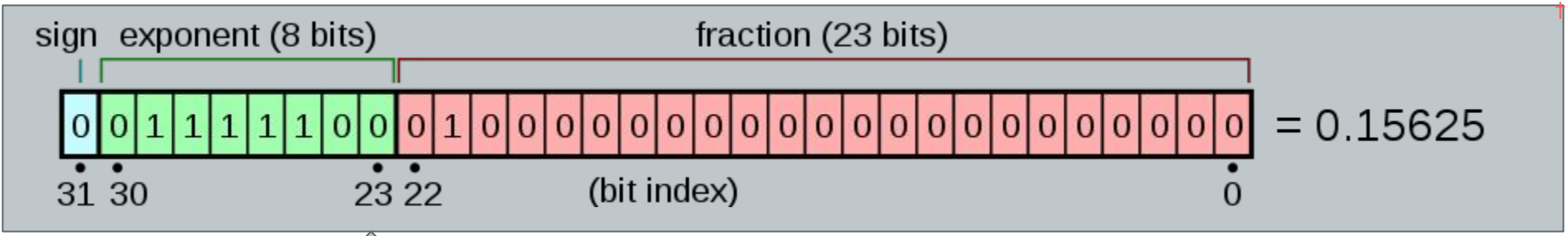

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Just like base 10 scientific notation, the exponent is shifted so that the first non-zero digit in the fraction is to the left of the decimal point. In binary, this value (2^{-0}=1) is implicit and not recorded. Since only the 2^{-2} bit is set above, the fraction value here is $2^{-0} + 2^{-2} = 1 + ¼ =$ **1.25**.

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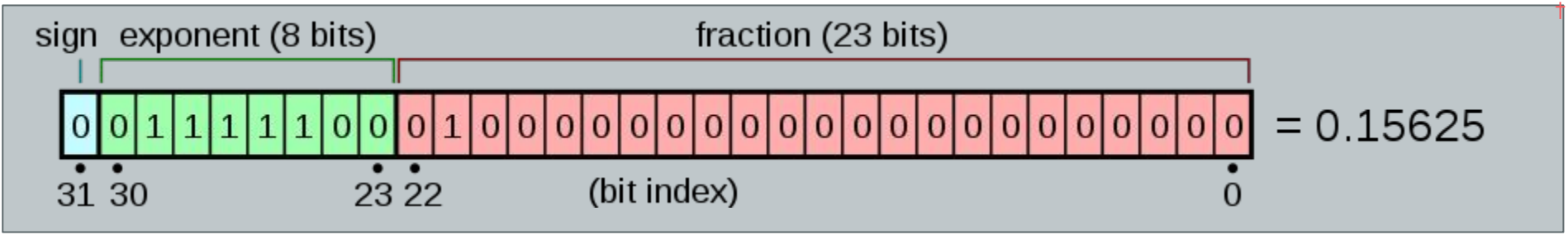

$$1 \times 2^{-3} \times 1.25 = 0.15625$$

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WHAT DOES IT MATTER? How does this affect my research?

- Machine precision is inherently limited
- This means rounding errors
- Rounding errors are a source of experimental error (in addition to modeling shortfalls) for computational science and can affect results
- Good research accounts for measurement error

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- Machine precision is inherently limited
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What can I do?

- Recognize the limitations of machine precision
- Make responsible and efficient choices regarding precision
  - AI/ML applications often use very low precision
  - GROMACS uses single precision by default
- Document choices
- Do better research

EXAMPLE: SUMMATION AND ROUNDING

$$1 + x \rightarrow 1 + x;\ x > \delta$$
$$1 + x \rightarrow 1;\ x <= \delta$$

$$y + x \rightarrow \max(x,y);\ x/y > \delta$$
$$y + x \rightarrow x + y;\ x/y <= \delta$$

SO WHAT IS THE ACTUAL LIMIT OF PRECISION for float32?

$$\log_{10} 2^{24} = 24 * \log_{10} 2 = \sim 7.2247$$

Just over seven decimal places.

EXERCISE: summing floats

```c
#include <stdio.h>

int main()
{
  float ttf = 16777216;   // 2^24
  float delta = 1.0f/ttf;  // 0.000000059604645
  float sum = 0.0f;

  // check inputs
  printf("Starting with sum=%1.18f, delta=%1.18f:\n\n", sum, delta);

  // should add to one
  for (int i=0; i<ttf; i++) sum += delta;
  printf("sum=%1.18f\n", sum);

  // what happens if we keep adding?
  for (int i=0; i<ttf; i++) sum += delta;
  printf("sum=%1.18f\n", sum);
}
```

EXERCISE: summing floats

```
discovery$ salloc -p debug -n 4 -c 4
…
node$ module load gcc/13.3.0 openmpi/5.0.5
node$ git clone https://github.com/frankwillmore/machine-numbers
node$ cd machine-numbers/machine_numbers_and_MPI
node$ vi add_float.c
node$ make add_float
node$ ./add_float
Starting with sum=0.000000000000000000, delta=0.000000059604644775:

sum=1.000000000000000000
sum=1.000000000000000000
```

EXERCISE: summing floats

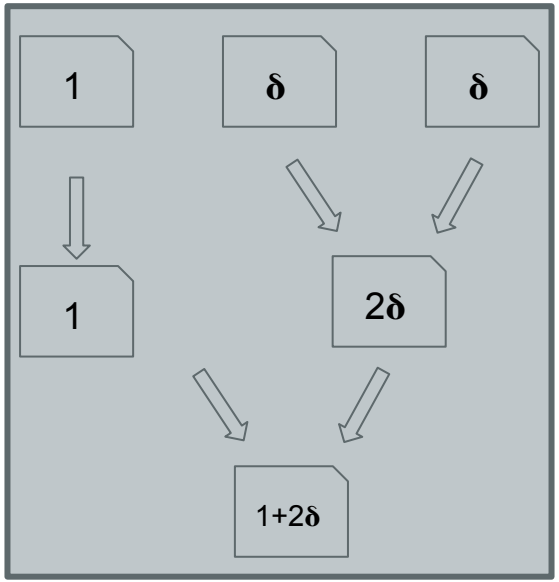
- What happens if you increase the size of ttf?
  - Edit add_float.c and recompile
  - What is the result?
- What happens if you decrease the size of ttf?
  - Edit add_float.c and attempt to recompile
  - What does the compiler say?
  - What does it mean?

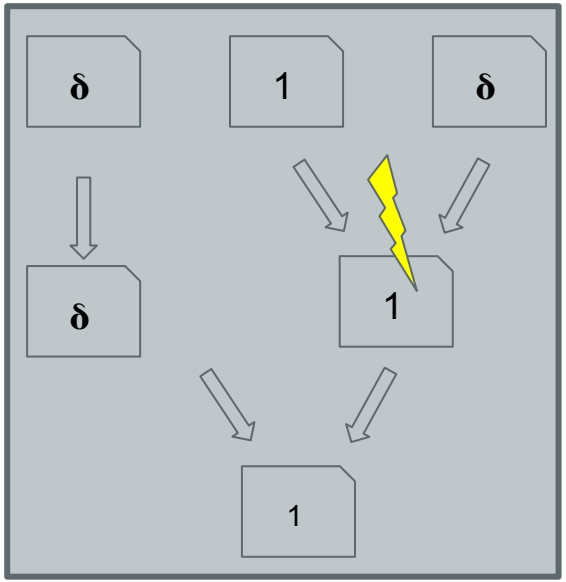
EXAMPLE OF MPI REDUCTION

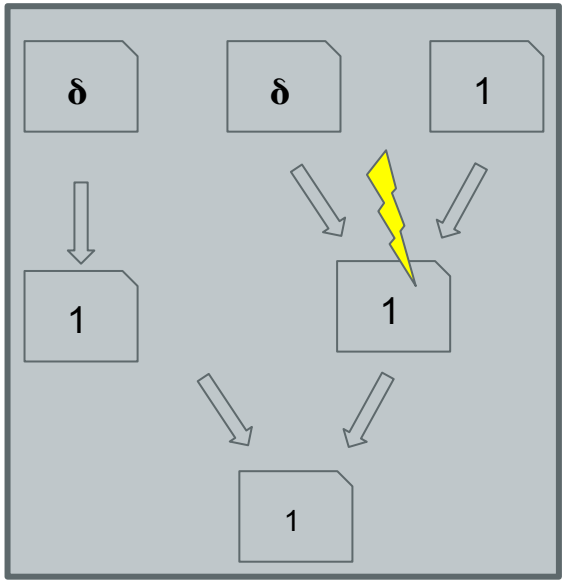
- MPI parallel processes run and complete in an indeterminate order
- Because of rounding, results of a reduction depend on the order in which operations are performed
- MPI operations can give results that vary between runs, depend on size of run, and even depend on which MPI you are using

EXAMPLE OF MPI REDUCTION

- MPI parallel processes run and complete in an indeterminate order
- Because of rounding(!), results of a reduction depend on the order in which operations are performed
- MPI operations can give results that vary between runs and depend on size of run







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EXERCISE: MPI reduction

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char* argv[])
{
  MPI_Init(NULL, NULL);

  float delta = 0.000000059604645;
  int mpi_rank, mpi_size;
  MPI_Comm_rank(MPI_COMM_WORLD, &mpi_rank);
  MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);

  for (int i=0; i<mpi_size; i++)
  {
    float global_sum, local_val;
    if (mpi_rank == i) local_val = 1.0f;
    else local_val = delta;
    MPI_Reduce(&local_val, &global_sum, 1, MPI_FLOAT, MPI_SUM, 0, MPI_COMM_WORLD);
    if (!mpi_rank) printf("big val to rank %d, gives global sum = %1.10f\n", i, global_sum);
  }

  MPI_Finalize( );
}
```

EXERCISE: MPI reduction

```
node$ vi reduce.c
node$ make reduce
node$ mpirun -n 3 ./reduce
rank 1/3 running.
rank 2/3 running.
rank 0/3 running.
big val to rank 0, gives global sum = 1.0000001192
big val to rank 1, gives global sum = 1.0000000000
big val to rank 2, gives global sum = 1.0000000000
```

EXERCISE: MPI reduction

- What happens if you run it again?
  - Do the processes still return in the same order?
  - What is the result?
- What happens if you increase the number of processes, e.g. to 4?
- What happens if you load a different MPI (e.g. mpich) and build/run?
  - Do OpenMPI and MPICH give the same results?
  - Why or why not?

EXAMPLE OF CENTRAL LIMIT THEOREM

The average values of sets of samples of a randomly distributed variable will tend to be distributed normally:

$\mathcal{R} \in [0,1)$; for a uniformly distributed random variable $\mathcal{R}$

$R_j \triangleq (1/N)\, \Sigma_i \mathcal{R}_i$; with average values R_j for sets of N samples of $\mathcal{R}$

$p(R_j) \propto \exp\{-(R_j - \langle R_j \rangle)^2/2\}$; those average values R_j are distributed normally

EXAMPLE OF CENTRAL LIMIT THEOREM

$\Re \in [0,1)$; for a uniformly distributed random variable $\Re$
$R_j \triangleq (1/N)\,\Sigma_i \Re_i$; with average values for a sets of N samples of $\Re$
$p(R_j) \propto \exp\{-(R_j - \langle R_j \rangle)^2/2\}$; those average values are distributed normally

The experiment:

- Using an MPI code with different random number seeds scattered to different MPI processes, sample values of R_j are generated and gathered.
- MPI parallel processes then run and complete, although in an indeterminate order
- Because of rounding, results of a reduction depend on the order in which operations are performed
- MPI operations can give results that vary between runs and depend on size of run

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EXERCISE: central limit theorem

```c
#include <stdio.h>
#include <mpi.h>
#include <math.h>
#include <stdlib.h>

int main(int argc, char* argv[])
{
  MPI_Init(NULL, NULL);

  int elements_per_proc = 8;
  int initial_seed = 123456;

  int mpi_rank, mpi_size;
  MPI_Comm_rank(MPI_COMM_WORLD, &mpi_rank);
  MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);

  if (!mpi_rank) printf("running %d elements per task with %d tasks.\n", elements_per_proc, mpi_size);

  // create seeds
  int scatter_seeds[mpi_size];
  scatter_seeds[0] = initial_seed;
  if (!mpi_rank) for (int i=1; i<mpi_size; i++) scatter_seeds[i] = scatter_seeds[0] + i;

  // scatter the seeds
  int seed;
  MPI_Scatter(scatter_seeds, 1, MPI_INT, &seed, 1, MPI_INT, 0, MPI_COMM_WORLD);
```

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EXERCISE: central limit theorem

```
// seed the RNG
srand(seed);

float sum = 0;
for (int i=0; i<elements_per_proc; i++)
{
  float sample = (float)rand() / (float)RAND_MAX;
  sum += sample;
}
sum /= elements_per_proc;

// gather and bin the results:
float results[mpi_size];
MPI_Gather(&sum, 1, MPI_FLOAT, results, 1, MPI_FLOAT, 0, MPI_COMM_WORLD);
```

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EXERCISE: central limit theorem

```
  int bins[10];
  for (int i=0; i<10; i++) bins[i] = 0;

  if (!mpi_rank) for (int i=0; i<mpi_size; i++)
  {
    printf("binning %f\n", results[i]);
    bins[(int)(results[i]*10)]++;
  }

  if (!mpi_rank) for (int i=0; i<10; i++)
  {
    for (int j=0; j<bins[i]; j++) printf("X");
    printf("\n");

  }
  MPI_Finalize();
}
```

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EXERCISE: central limit theorem

```
node$ vi central_limit.c
node$ make central_limit
node$ mpirun -n 48 ./central_limit
running 8 elements per task with 48 tasks.
binning 0.488702
binning 0.511513
. . .


XX
XX
XXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXX
XXXXXXXX
XX
X
```

EXERCISE: central limit theorem

- What are the likely sources of error and uncertainty?
- What happens if you run it again for a different seed value?
- What happens if you increase the number of MPI processes?
- What happens if you use a different number of samples for each R_j?
- What happens if we have very small values of $\mathcal{R}$?

TAKEAWAY POINTS

- Greater precision isn't always 'better'
- Knowing when you can use a smaller type can often mean better performance
- Making good choices here depends on understanding the limits of machine numbers
- Operations can give results that vary between runs and depend on size of run
- 'Randomness' is not always an implicit source of error, it depends on how it's used.
- There is a new floating point standard in play (posits) which looks to gain traction
- Limits of machine precision are inherent, no matter the standard

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Wait, there's more!

BONUS TOPIC! CUDA/GPU application

- Q: When is it a good idea to use a GPU?
- A: For anything that looks (or can look) like a rendering problem.

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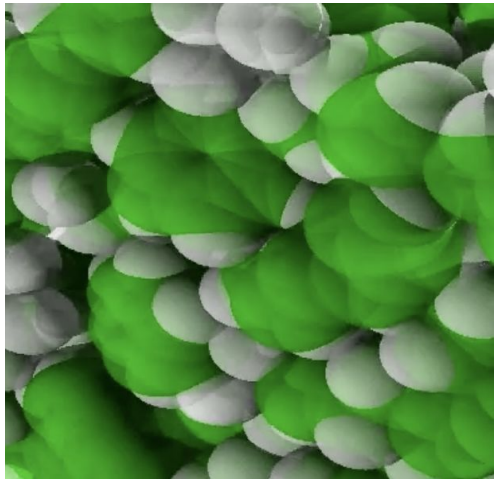

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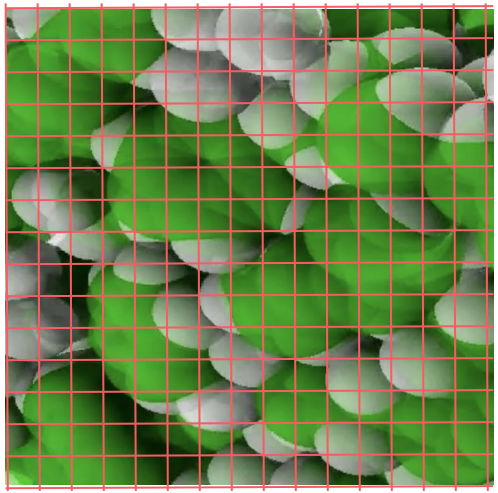
Domain decomposition



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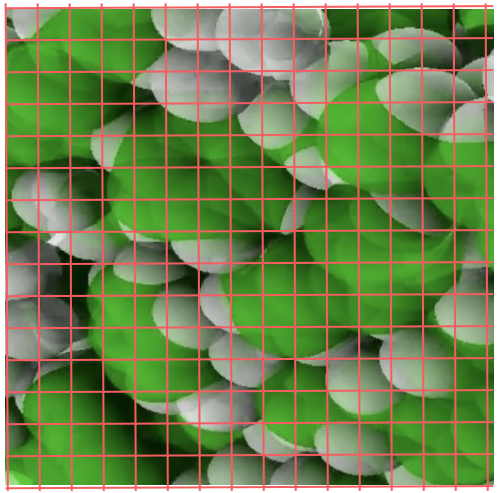

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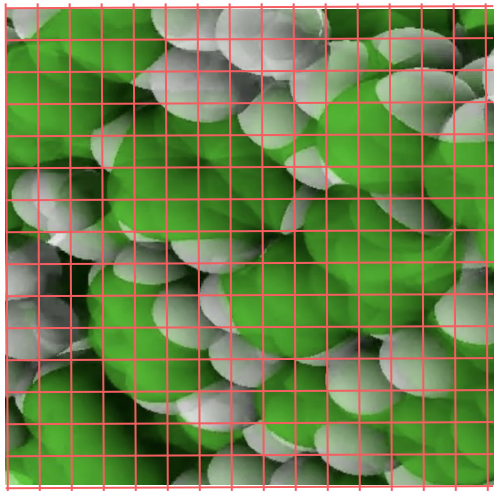

Chemical potential:

$$\mu_i = \left(\frac{\partial U}{\partial N_i}\right)_{S,V,N_{j\neq i}} \cdot \quad \mu_i = -k_B T \ln\left(\frac{\mathbf{B}_i}{\rho_i \lambda^3}\right)$$

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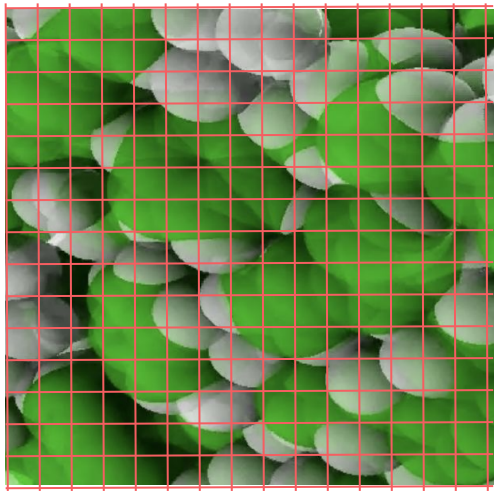

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Wisdom insertion parameter:

$$\mathbf{B}_i = \frac{\rho_i}{a_i} = \left\langle \exp\left(-\frac{\psi_i}{k_B T}\right)\right\rangle$$

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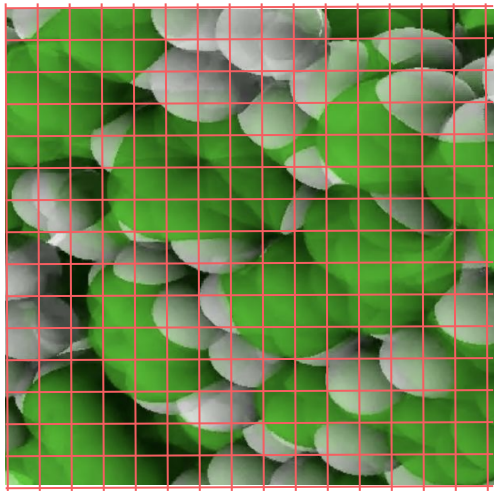

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Free volume index:

$$\phi_i(x,y,z) = e^{-\beta\gamma_i}$$

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EXERCISE: free volume *via* GPU

```
discovery$ salloc --partition=gpu --gres=gpu:1 \
                  --cpus-per-task=4 --mem=32GB \
                  --time=1:00:00
node$ module load vacuumms
node$ cd ~/machine-numbers/GPU_fun
node$ head PS.gfg
33.637309   36.915309   35.467309   3.520530    0.073457
36.121309   38.629309   34.794309   2.373410    0.028294
34.127309   39.183309   34.275309   3.581180    0.066301
33.785309   38.464309   35.581309   3.581180    0.066301
39.593309   33.823309   36.362309   2.373410    0.028294
33.439309   38.942309   33.477309   2.373410    0.028294
35.546309   38.832309   33.826309   3.581180    0.066301
35.729309   40.915309   33.360309   2.373410    0.028294
34.054309   40.296309   34.378309   2.373410    0.028294
34.658309   38.544309   36.220309   2.373410    0.028294
node$ ./rungfg2fvi.sh &
reading configuration
calculating resolution = 256 for 612 potential
using sigma = 0.000000 and epsilon = 1.000000
node$
```

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EXERCISE: free volume *via* GPU

```
node$ nvidia-smi
Thu Mar 23 11:17:06 2023
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.39.01    Driver Version: 510.39.01    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-PCIE...  On   | 00000000:3B:00.0 Off |                  Off |
| N/A   47C    P0   215W / 250W |   1365MiB / 16384MiB |    100%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
|   1  Tesla V100-PCIE...  On   | 00000000:D8:00.0 Off |                  Off |
| N/A   30C    P0    23W / 250W |      4MiB / 16384MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A     99430      C   gfg2fvi                         1361MiB |
+-----------------------------------------------------------------------------+
username@gpuxxx$
```

WRAP-UP

Interesting GPU fact:

- The first GPUs didn't perform compliant arithmetic operations
- IEEE Compliant operations require:
  - padding 32 bit float to a 40 bit type
  - Performing arithmetic on 40 bit type
  - Rounding the result back to a 32 bit type
- Since they were only shading pixels, a little round-off error didn't matter much

Additional resources:

- https://en.wikipedia.org/wiki/IEEE_754
- https://posithub.org/docs/posit_standard-2.pdf
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