
OAK RIDGE National Laboratory

SC25 ST. LOUIS NOV 16–21

# ChatHPC:
## Building the foundation of an AI assisted and productive HPC ecosystem









**PRESENTED BY**

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# ChatHPC, What is that?

## Infrastructure:

- A CLI Python library on top of:
  - Code Llama, PyTorch, and LoRA
- The ChatHPC library makes:
  - Fine-tuning, Testing, Refinement, Merge, and Inference

## Ecosystem:

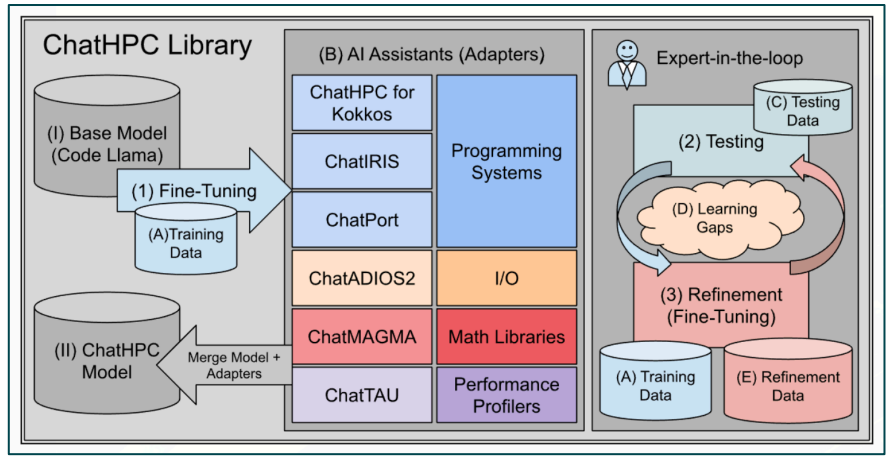
- A collection of AI assistants leveraging existing HPC efforts for multiple domains:
  - Programming Models, Math Libraries, I/O, Tooling, etc.
- And priorities:
  - Parallelization, Portability, Optimization, Evaluation, etc.

ChatHPC CLI:

```
$ chathpc train   # Finetune the assistent.
$ chathpc verify  # Verify the assistent on training set.
$ chathpc test    # Test the asssistent on unseen data.
$ chathpc run     # Interactivly run the assistent.
```

Interactive Run Session:

```
$ chathpc ()> /context
Context: Introduction to Kokkos
$ chathpc (Introduction to Kokkos)> What is LayoutLeft?
LayoutLeft refers column-major layout where consecutive entries in
      the same column of a 2-D array are contiguous in memory.
```

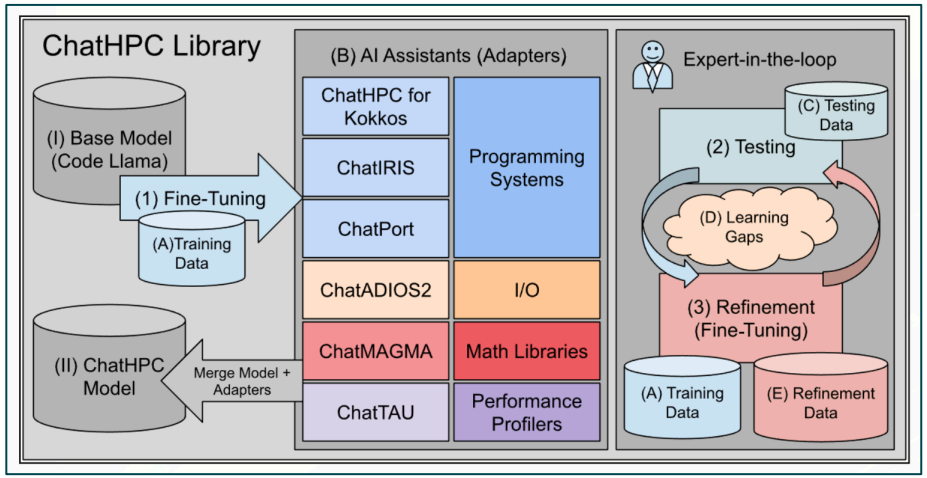


# Design and Implementation

A simple 3-step iterative process:

1. Fine-tuning -> AI assistant (optimizers)
   - Training Data
   - The better the data the better the model
   - It is more about quality than quantity
2. Testing -> Learning gaps
   - Testing Data != Training Data
   - Testing Data may contain question about non-fined-tuned capabilities
3. Refinement -> More capable AI assistants
   - Expert-Supervised Refinement Data

AI assistants can be merge into a single LLM: ChatHPC model




```
[
 {"question": "Can you translate this HIP code to Kokkos?
  __global__ void stencil (int n, float dx, float dy, float *u,
      float *u_new, float *f) {
    int i = blockIdx.x * blockDim.x + threadIdx.x;
    int j = blockIdx.y * blockDim.y + threadIdx.y;
    if(i > 0 && i < n-1 && j > 0 && j < n-1){
     u_new[i][j] = 0.25 * (u[i-1][j] + u[i][j+1]
                 + u[i][j-1] + u[i+1][j] + f[i][j]);
    }
  }",
  "context": "HIP to Kokkos translation",
  "answer":
  "Kokkos::parallel_for(\"stencil\",
     Kokkos::MDRangePolicy<Kokkos::Rank<2>>
              ({1, 1}, {n-1, n-1}),
     KOKKOS_LAMBDA(const int i, const int j) {
      u_new(i,j) = 0.25 * (u(i-1,j) + u(i,j+1)
                 + u(i,j-1 + u(i+1,j) + f(i,j));
  });"
  },
  ...
]
```

# Analysis

- Code Llama 7B [13GB]
  - ChatGPT 4o 1.8T -> 257x less parameters
- AI assistants (~100MB)
- Training data (~KB)
- Evaluation data (~KB)
- Fine-tuning:
  - No more than 15 min. in a one NVIDIA 2x H100 node
- Evaluation
  - % of prompts (evaluation data) passed
  - Evaluation data is different to training data
- Compare against
  - 7 billion parameter Meta's Code Llama base model (no fine-tuning)
  - 1.8 trillion parameter OpenAI's ChatGPT 4o model

- Data
  - Synthetic data in most of the AI-assistants created (supervised learning)
    - Kernels
    - Applications
    - Scripts
  - Applications:
    - Dense/Sparse Linear Algebra, PDEs, CFD, AI, Image Processing, …
  - Expert-in-the-loop
    - If we want AI responding as expert, we need data provided by experts
    - Create data
    - Identify learning gaps
  - Minimize data demanding
  - Self-learning
  - Reinforcements, if necessary (learning gaps)
  - Which targets are more demanding?
  - Not use all data (training data) we can use

# ChatHPC for Kokkos

| Model/Context | CodeLlama | ChatHPC for Kokkos Initial | ChatHPC for Kokkos Refinement | ChatGPT |
|---|---|---|---|---|
| **Documentation** | 9.5% | **89.0%** | - | 81.0% |
| **Installation** | 27.2% | **78.0%** | - | 45.5% |
| **Development** | 0.0% | **85.0%** | - | 15.1% |
| **Parallelization** | 0.0% | 45.5% | **90.9%** | 66.7% |
| **Portability** | 0.0% | 55.6% | **85.9%** | 33.4% |
| **CUDA*** | 0.0% | 53.2% | **87.2%** | 41.3% |
| **OpenACC*** | 0.0% | 58.7% | **83.5%** | 31.2% |

Kokkos: A C++ API portable library for parallel programming

Parallelization and Portability

- Training (HPC and scientific kernels)
  - BLAS, Sparse, Euler methods, Conjugate Gradient, LBM, AI convolutions
- Learning gaps
  - Sparse Computation and Iterative Solvers
  - 12% more data

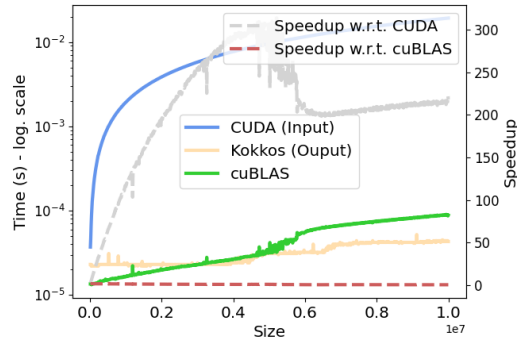
No CUDA and OpenACC codes used for fine-tuning

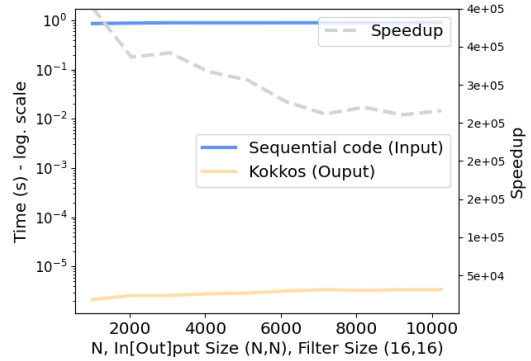
Translate the next CUDA code to Kokkos:

```
__global__ void sdot(int n, float *x, float *y, float *result) {
  int i = threadIdx.x + blockIdx.x * blockDim.x;
  float update = 0.0;
  if (i < SIZE) {
    update = x[i] * y[i];
    atomicAdd(result, update);
  }
}
```

*ChatKokkos* output:

```
Kokkos::parallel_reduce(SIZE,
  KOKKOS_LAMBDA(int i, float &update){
    update += x(m) * y(m);
  },
  Kokkos::Sum<float>(result));
```



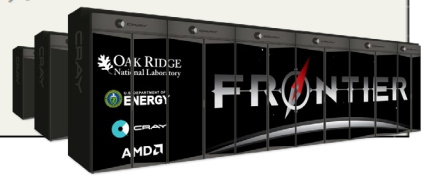



# ChatADIOS2

| Model/Context | CodeLlama | ChatADIOS2 Intial | ChatADIOS2 Refinement | ChatGPT |
|---|---|---|---|---|
| **Introduction** | 0.0% | 77.0% | **100.0%** | 33.3% |
| **Variable Definition** | 0.0% | 50.0% | **100.0%** | 33.3% |
| **Data Compression** | 0.0% | 25.0% | **100.0%** | 0.0% |
| **Parallelization** | 0.0% | 0.0% | **100.0%** | **100.0%** |

```
adios2::ADIOS adios("adios2_config.yaml", mpiComm);
adios2::IO io = adios.DeclareIO("WriteIO");
adios2::Variable<double> varU =
      io.DefineVariable<double>("U",shape,start,count);
adios2::Operator Zfp =
      adios.DefineOperator("Zfp", adios2::ops::LossyZFP);
varU.AddOperation(Zfp,{{adios2::ops::zfp::key::rate,"9"}});

adios2::Engine bpWriter =
      io.Open("output.bp", adios2::Mode::Write);
while( run_simulation ){
      bpWriter.BeginStep();
      bpWriter.Put<double>(varU, U.data());
      ...
      bpWriter.EndStep();
}
bpWriter.Close();
```



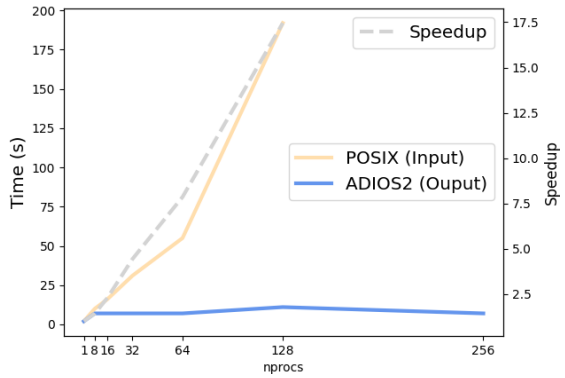

ADIOS2: A portable and HPC I/O library

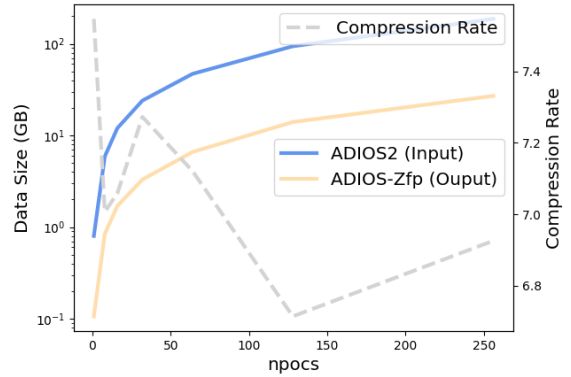
Capabilities:

- Q&A on API, Variable definition, Compression, and Parallelization (serial POSIX I/O to ADIOS2)

Learning gaps:

- Wrong use of ADIOS2 API
  - Local and global N-dimension variables
  - Compression factor (parameters)



# ChatIRIS

| Model/Context | CodeLlama | ChatIRIS Intial | ChatGPT |
|---|---|---|---|
| **Documentation** | 0.0% | **95.0%** | 70.0% |
| **OpenMP -> IRIS** | 0.0% | **82.5%** | 10.0% |
| **CUDA -> IRIS** | 0.0% | **90.0%** | 50.0% |
| **HIP -> IRIS*** | 0.0% | **81.6%** | 10.0% |

IRIS: A Task-based programming model for heterogeneous computing

- Taskification of applications
  - Deploy applications on any architecture using multiple devices
- Portability
  - OpenMP, CUDA, HIP to IRIS task code
- Training
  - Basic applications (AXPY)
- Testing
  - More complex applications with multiple kernel invocations
- No refinements were needed
- HIP was not used for fine-tuning

Translate the next CUDA code to IRIS:

```
alpha = 2.0;
X = (float *) malloc(SIZE * sizeof(float));
Y = (float *) malloc(SIZE * sizeof(float));
Z = (float *) malloc(SIZE * sizeof(float));
for (int i = 0; i < SIZE; i++) { X[i] = i; Y[i] = i;}
cudaMalloc((void**)&d_x, SIZE * sizeof(float));
cudaMalloc((void**)&d_y, SIZE * sizeof(float));
cudaMalloc((void**)&d_z, SIZE * sizeof(float));
// Initialization of arrays
cudaMemcpy(d_x, x, SIZE* sizeof(float), cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, SIZE* sizeof(float), cudaMemcpyHostToDevice);
int threads = 512;
int blocks = floor(SIZE/threads) + 1;
saxpy<<<blocks, threads>>>(alpha, d_x, d_y, SIZE);
cudaDeviceSynchronize()
sdot<<<blocks, threads>>>(d_z, d_x, SIZE);
cudaDeviceSynchronize()
cudaMemcpy(z, d_z, SIZE * sizeof(float), cudaMemcpyDeviceToHost);
cudaFree(d_x);
cudaFree(d_y);
cudaFree(d_z);
free(X);
free(Y);
free(Z);
```

*ChatIRIS* output:

```
// Architecture-agnostic IRIS task code
alpha = 2.0;
iris_init(&argc, &argv, 1);
iris_mem iris_x;
x = (float *) malloc(SIZE * sizeof(float));
iris_data_mem_create(&iris_x, x, SIZE * sizeof(float));
iris_mem iris_y;
y = (float *) malloc(SIZE * sizeof(float));
iris_data_mem_create(&mem_Y, Y, SIZE * sizeof(float));
iris_mem iris_z;
z = (float *) malloc(SIZE * sizeof(float));
iris_data_mem_create(&mem_z, z, SIZE * sizeof(float));
// Initialization of arrays
iris_graph graph;
iris_graph_create(&graph);
iris_task saxpy_task;
iris_task sdot_task;
iris_task_create(&saxpy_task);
iris_task_create(&sdot_task);
void* saxpy_params[3]={&alpha, &iris_x, &iris_y};
int saxpy_params_info[3]={sizeof(A), iris_w, iris_r};
iris_task_kernel(task0, "saxpy", 1, NULL, &SIZE, NULL, 3,
      saxpy_params, saxpy_params_info);
void* sdot_params[2]={&iris_z, &iris_x};
int sdot_params_info[2]={iris_w, iris_r};
iris_task_kernel(task1, "sdot", 1, NULL, &SIZE, NULL, 2,
      sdot_params, sdot_params_info);
iris_graph_task(graph, saxpy_task, iris_default, NULL);
iris_graph_task(graph, sdot_task, iris_default, NULL);
iris_graph_submit(graph,iris_any,1);
free(X);
free(Y);
free(Z);
iris_finalize();
```

# ChatMAGMA

| Model/Context | CodeLlama | ChatMAGMA Initial | ChatMAGMA Refinement | ChatGPT |
|---|---|---|---|---|
| **MKL -> MAGMA** | 0.0% | 37.5% | **93.0%** | 0.0% |
| **cuBLAS/Solver -> MAGMA** | 0.0% | 50.0% | **96.5%** | 0.0% |
| **hipBLAS/Solver -> MAGMA** | 0.0% | 45.3% | **95.3%** | 0.0% |

MAGMA: A portable (CPU+GPU) BLAS and LAPACK library with +400 routines

Capabilities:

- Porting of vendor (arch)-specific applications to MAGMA
  - Support for heterogeneous (CPU+ GPU) computing
- Training
  - Well known BLAS (dgemm, dtrsm) and LAPACK (dgetsv, dpotrf) for double precision
- Testing
  - Rest of BLAS and LAPACK for other precisions
- Learning gaps:
  - MAGMA-specific data types (queues) for different precisions
  - 51.72% extra data

No AMD math libraries codes were used for fine-tuning

Translate the next Intel MKL code to MAGMA:

```
// Intel MKL (CPU-only) dgetrf code
double *A=(double *)mkl_malloc(n*n*sizeof(double),64);
int *ipiv=(int *)mkl_malloc(n*sizeof(int),64);
LAPACKE_dgetrf(LAPACK_ROW_MAJOR,n,n,A,n,ipiv);
mkl_free(A);
mkl_free(ipiv);
```

Translate the next NVIDIA cuSolver code to MAGMA:

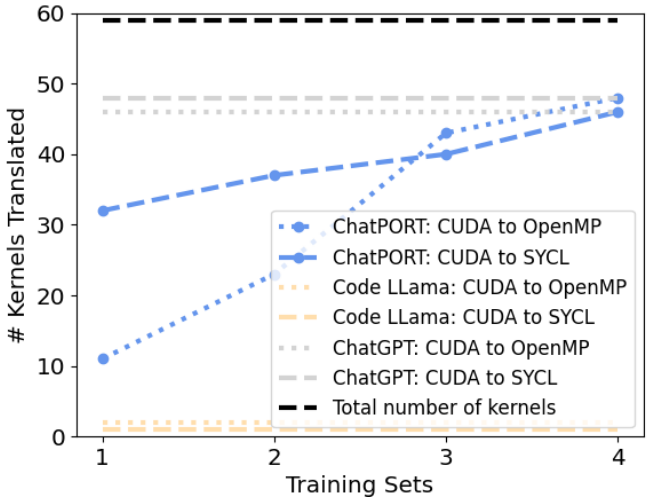
```
// NVIDIA cuSolver (GPU-only) dgetrf code
int lwork=0;
double *dwork;
int *dipiv;
double *dinfo;
cusolverDnHandle_t handle;
cusolverDnCreate(&handle);
double *hA=(double *)malloc(n*n*sizeof(double));
cusolverDnDgetrf_bufferSize(handle,n,n,dA,n,&lwork));
cudaMalloc((void **)&dA,n*n*sizeof(double));
cudaMalloc((void **)&dwork,sizeof(double)*lwork);
cudaMalloc((void **)&dipiv, n*sizeof(int));
cudaMalloc((void **)&dinfo,sizeof(int));
cudaMemcpy(dA,hA,n*n*sizeof(double),cudaMemcpyHostToDevice);
cusolverDnDgetrf(handle,n,dA,n,dwork,dipiv,dinfo);
cudaMemcpy(hA,dA,n*n*sizeof(double),cudaMemcpyDeviceToHost);
cudaFree(dA);
cudaFree(dwork);
cudaFree(dipiv);
cudaFree(dinfo);
free(hA);
cusolverDnDestroy(handle);
```

*ChatMAGMA* output:

```
// MAGMA (CPU+GPU) dgetrf code
magma_queue_t queue;
magma_device_t cdev;
magma_getdevice(&cdev);
magma_queue_create(cdev,&queue );
double *hA;
magmaDouble_ptr dA;
magma_int_t *ipiv;
magma_int_t info;
magma_dmalloc_cpu(&hA,n*n);
magma_dmalloc(&dA,n*n);
magma_imalloc_cpu(&ipiv,n);
magma_dsetmatrix(n,n,hA,n,dA,n,queue);
magma_dgetrf_gpu(n,n,dA,n,ipiv,&info);
magma_dgetmatrix(n,n,dA,n,hA,n,queue);
magma_free(dA);
magma_free_cpu(hA);
magma_free_cpu(ipiv);
magma_queue_destroy(queue);
```

# ChatPORT(ing)

| Training Set | #Kernels | Kernels |
|---|---|---|
| 1 | 5 | accuracy, geodesic, lr, maxpool3d, perplexity |
| 2 | 10 | damage, knn, heat2d, laplace3d, md |
| 3 | 15 | advCubatureHex3D, backprop, channelShuffle, lr, meanshift |
| 4 | 22 | chemv, clenergy, pathfinder, pointwise, swish, stddev, tissue |




- Create an AI assistant for code portability from vendor-specific models (e.g., CUDA) to SYCL and OpenMP-offloading
- Data is provided by HeCBench
  - Training:
    - 4 different data sets with (5, 10, 15, and 22) kernels from multiple different domains
  - Testing
    - 59 CUDA kernels to be ported to OpenMP-offloading and SYCL

# Remarks

| Assistant | Code Llama | Initial | Extra Data | Refinement | ChatGPT |
|---|---|---|---|---|---|
| **ChatHPC for Kokkos** | 7.34% | 70.51% | 12.33% | **85.75** | 48.34% |
| **ChatADIOS2** | 0.00% | 40.87% | 37.50% | **100.00%** | 25.0% |
| **ChatMAGMA** | 0.00% | 44.26% | 51.72% | **94.93%** | 0.00% |
| **ChatIRIS** | 0.00% | **87.29%** | - | - | 35.00% |
| **ChatPort** | 2.54% | 36.44% | 77.27% | **79.66%** | **79.66%** |

- New HPC-specific capabilities on top of Code Llama across different HPC domains
  - Programming models, I/O, math libraries, tooling, and runtimes

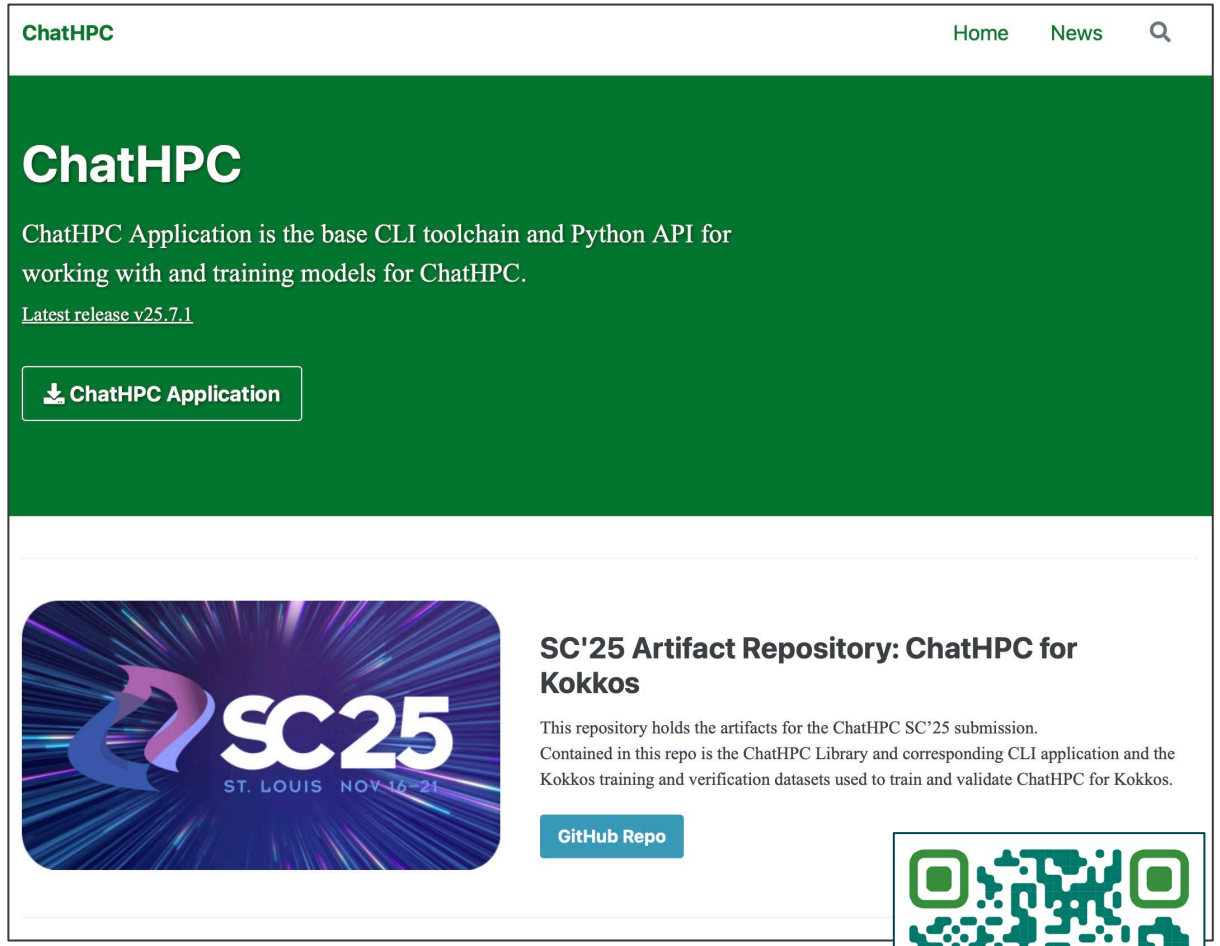
  And tasks:
  - Parallelization, portability, performance analysis, scalability, etc.
- Provide higher levels (of up to 90% higher) of trustworthiness than ChatGPT quickly with modest resources
  - Increase data-size (expert-in-the-loop) during refinement learning has a higher impact on correctness
- More data (prompts) for testing than for training data
  - Testing data contains prompts about non-fine-tuned capabilities

# Future Work

- **ChatMPI**
  - A ChatHPC AI-assistant for MPI parallelization
    - 4x speedup w.r.t. MPI code generated by ChatGPT-5
- **3 Pillars**
  - **Multimodality**
    - Simplify the interaction with AI for HPC domains
  - **Reasoning**
    - Generate highly optimized HPC codes across domains and technologies
  - **Agentic**
    - Connect HPC and AI for complex problems

# Resources and Community

- ChatHPC project:
  https://ornl.github.io/ChatHPC/
- Meetings:
  - We organize a community meeting once a month.
  - Join us!
- Workshops:
  - LLM4HPC (co-located with ISC-HPC):
    https://ornl.github.io/events/llm4hpc2025/
  - LLM4HPCAsia (collocated with SCA/HPC Asia)
    https://ornl.github.io/events/llm4hpcasia2026/



# Observations (Things to think about)

- **Fine-tuning**
  - Very effective, if you have the data
- **Trustworthiness**
  - You can elevate trustworthiness (BTW: better than ChatGPT)
- **Overfitting**
  - Is that a problem for domain-specific AI assistants?
- **Self-learning**
  - Train on simple problems and let LLMs to deal with more complex problems
  - Take advantage from similarities (similar patterns)
- **Synthetic or real data?**
  - Why not both?
- **Expert-in-the-loop**
  - Recommendable for domain-specific LLMs
- **Accessibility**
  - One NVIDIA GPU (better if you have 2), data (~KB), and 15 minutes
- **Simplify prompting**
  - No prompt engineering, more productive, non-experts can generate expert level responses
- **Impact on HPC**
  - Created capabilities for programming models, I/O, math libraries, performance tools, …
  - **Help our community to use the HPC tools we have today**
- **Leveraging HPC efforts**
  - ChatHPC benefits from the big effort made during last years

# Use ChatHPC!

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SC25 ST. LOUIS NOV 16–21

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# Thanks!


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