

# MAKING PARALLEL COMPUTING AS EASY AS PY(THON), FROM LAPTOPS TO SUPERCOMPUTERS

Brad Chamberlain, distinguished technologist HPE Dev Munch & Learn April 20, 2022



# **PARALLEL COMPUTING BASICS**

# Q: What is parallel computing?

A: Running an application using multiple processors in order to...

...run it faster and/or...

...run it using larger data sets...

...than you could with just a single processor.

### HPC =

High Performance Computing (parallel computing at the largest scales)

# Q: Where can I run parallel programs?

**A:** These days, everywhere:

- multi-core processors in laptops
- commodity clusters
- the cloud
- enterprise servers and supercomputers
  - HPE Apollo, HPE Superdome Flex, HPE Cray EX, ...





# Q: What are the main barriers to doing parallel computing?

A: Writing parallel programs is challenging by nature—and even more so for distributed memory systems



# PARALLEL COMPUTING THAT'S AS EASY AS PYTHON?

Imagine having a programming language for parallel computing that was as...

...**programmable** as Python

```
...yet also as...

...fast as Fortran

...scalable as MPI or SHMEM

...portable as C

...flexible as C++

...type-safe as Fortran, C, C++, ...

...fun as [your favorite programming language]
```

This is the motivation for the Chapel language

# WHAT IS CHAPEL?

# Chapel: A modern parallel programming language

- portable & scalable
- open-source & collaborative



# **Goals:**

- Support general parallel programming
- Make parallel programming at scale far more productive

# WHAT DO CHAPEL PROGRAMS LOOK LIKE?

**helloTaskPar.chpl:** print a message from each core in the system

```
> chpl helloTaskPar.chpl
> ./helloTaskPar --numLocales=4
Hello from task 1 of 4 on n1032
Hello from task 4 of 4 on n1032
Hello from task 1 of 4 on n1034
Hello from task 2 of 4 on n1032
Hello from task 1 of 4 on n1033
Hello from task 3 of 4 on n1034
...
```

**fillArray.chpl:** declare and initialize a distributed array

```
use CyclicDist;
config const n = 1000;
const D = {1..n, 1..n}
          dmapped Cyclic(startIdx = (1,1));
var A: [D] real;
forall (i,j) in D do
    A[i,j] = i + (j - 0.5)/n;
writeln(A);
```

```
> chpl fillArray.chpl
> ./fillArray --n=5 --numLocales=4
1.1 1.3 1.5 1.7 1.9
2.1 2.3 2.5 2.7 2.9
3.1 3.3 3.5 3.7 3.9
4.1 4.3 4.5 4.7 4.9
5.1 5.3 5.5 5.7 5.9
```

# **KEY CHARACTERISTICS OF CHAPEL**

- **compiled:** to generate the best performance possible
- statically typed: to avoid simple errors after hours of execution
- interoperable: with C, Fortran, Python, ...
- **portable:** runs on laptops, clusters, the cloud, supercomputers
- open-source: to lower barriers to adoption and leverage community contributions

# **CHAPEL RELEASES**

# Q: What is provided in a Chapel release?

A: Chapel releases contain...

...the Chapel compiler ('chpl'): translates Chapel source code into optimized executables

...runtime libraries: help map Chapel programs to a system's capabilities (e.g., processors, network, memory, ...)

...library modules: provide standard algorithms, data types, capabilities, ...

...documentation: also available online at: <a href="https://chapel-lang.org/docs/">https://chapel-lang.org/docs/</a>

...**sample programs:** primers, benchmarks, etc.

# Q: How often is Chapel released? When is the next one?

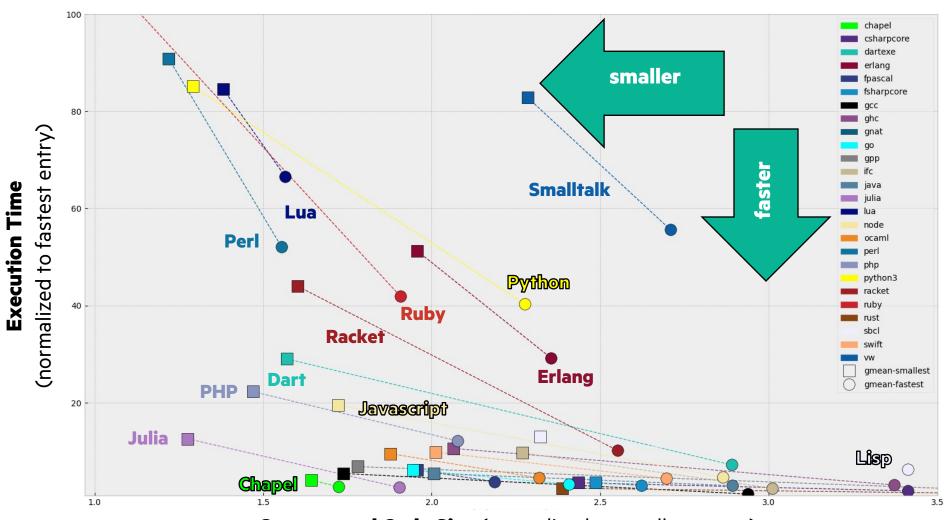
A: New Chapel releases are made available every 3–6 months

version 1.26.0 was released March 31, 2022

# HOW DOES CHAPEL COMPARE TO OTHER PROGRAMMING LANGUAGES?

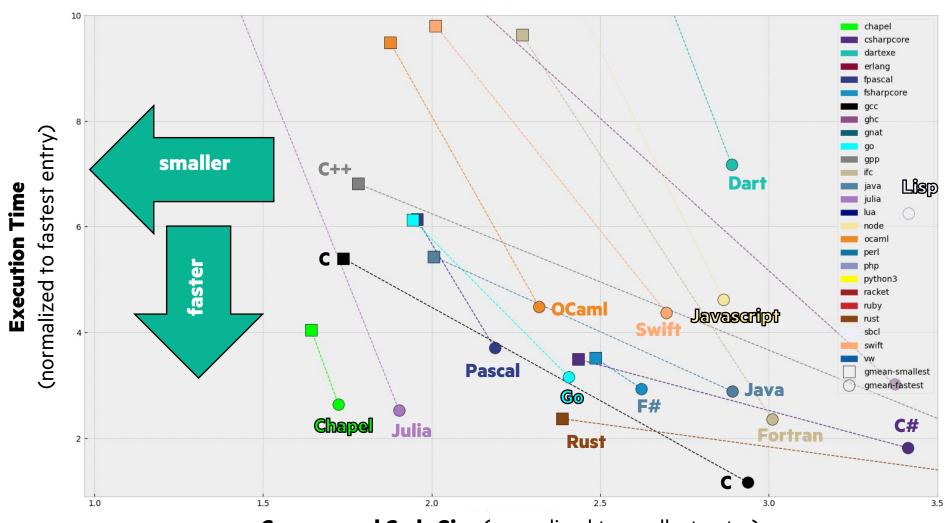


# FOR DESKTOP BENCHMARKS, CHAPEL TENDS TO BE COMPACT AND FAST



**Compressed Code Size** (normalized to smallest entry)

# FOR DESKTOP BENCHMARKS, CHAPEL TENDS TO BE COMPACT AND FAST



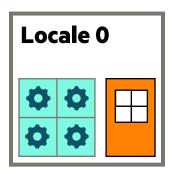
**Compressed Code Size** (normalized to smallest entry)

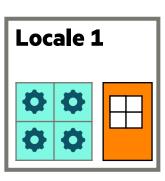
# HOW DOES CHAPEL COMPARE TO PROGRAMMING APPROACHES USED FOR HPC?



# **KEY CONCERNS FOR SCALABLE PARALLEL COMPUTING**

- **1. parallelism:** What tasks should run simultaneously?
- **2. locality:** Where should tasks run? Where should data be allocated?









Processor Core

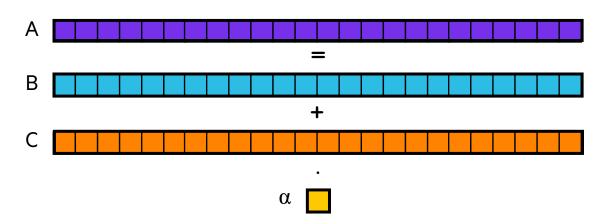
Memory



**Given:** *m*-element vectors *A*, *B*, *C* 

**Compute:**  $\forall i \in 1..m, A_i = B_i + \alpha \cdot C_i$ 

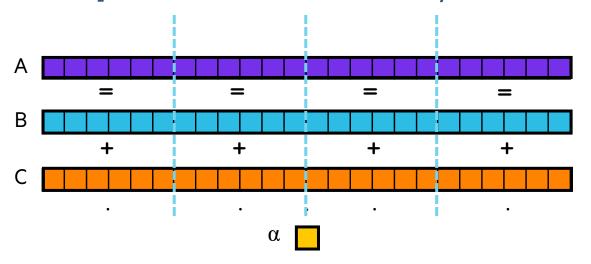
# In pictures:



**Given:** *m*-element vectors *A*, *B*, *C* 

**Compute:**  $\forall i \in 1..m, A_i = B_i + \alpha \cdot C_i$ 

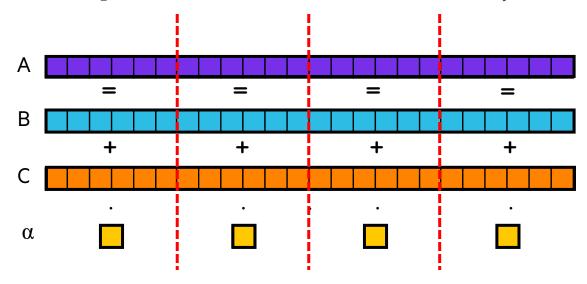
In pictures, in parallel (shared memory / multicore):



**Given:** *m*-element vectors *A*, *B*, *C* 

**Compute:**  $\forall i \in 1..m, A_i = B_i + \alpha \cdot C_i$ 

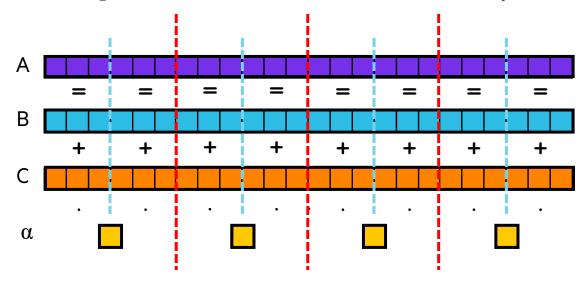
In pictures, in parallel (distributed memory):



**Given:** *m*-element vectors *A*, *B*, *C* 

**Compute:**  $\forall i \in 1..m, A_i = B_i + \alpha \cdot C_i$ 

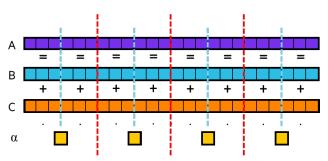
In pictures, in parallel (distributed memory multicore):





# STREAM TRIAD IN CONVENTIONAL HPC PROGRAMMING MODELS

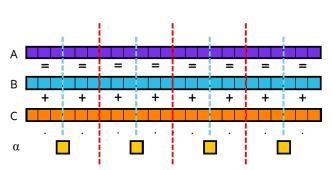
Many Disparate Notations for Expressing Parallelism + Locality



```
#include <hpcc.h>
                                                       if (!a || !b || !c) {
                                                        if (c) HPCC free(c);
                                                        if (b) HPCC free(b);
                                                        if (a) HPCC free(a);
                                                        if (doIO) {
static int VectorSize;
                                                          fprintf( outFile, "Failed to
static double *a, *b, *c;
                                                             allocate memory (%d).\n",
                                                            VectorSize );
int HPCC StarStream(HPCC Params *params) {
                                                          fclose( outFile );
 int myRank, commSize;
 int rv, errCount;
                                                        return 1;
 MPI Comm comm = MPI COMM WORLD;
 MPI Comm size ( comm, &commSize );
 MPI Comm rank ( comm, &myRank );
  rv = HPCC Stream( params, 0 == myRank);
                                                      for (j=0; j<VectorSize; j++) {</pre>
 MPI_Reduce( &rv, &errCount, 1, MPI_INT, MPI_SUM,
                                                        b[j] = 2.0;
   0, comm);
                                                        c[j] = 1.0;
 return errCount;
                                                      scalar = 3.0;
int HPCC Stream(HPCC Params *params, int doIO) {
 register int j;
 double scalar;
                                                      for (j=0; j<VectorSize; j++)</pre>
                                                        a[i] = b[i] + scalar * c[i];
 VectorSize = HPCC LocalVectorSize( params, 3,
   sizeof(double), 0);
                                                      HPCC free(c);
                                                      HPCC free (b);
 a = HPCC XMALLOC( double, VectorSize );
                                                      HPCC_free(a);
 b = HPCC XMALLOC( double, VectorSize );
 c = HPCC XMALLOC( double, VectorSize );
                                                      return 0; }
```

# STREAM TRIAD IN CONVENTIONAL HPC PROGRAMMING MODELS

Many Disparate Notations for Expressing Parallelism + Locality



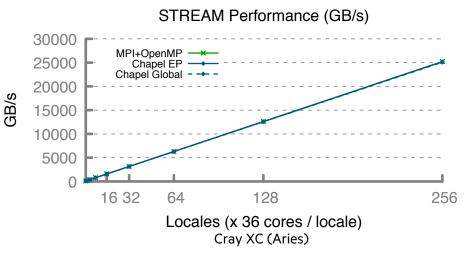
```
MPI + OpenMP
                                                       if (!a || !b || !c) {
#include <hpcc.h>
                                                                                          #define N 2000000
                                                                                                                    CUDA
#ifdef OPENMP
                                                         if (c) HPCC free(c);
                                                         if (b) HPCC free(b);
                                                                                          int main() {
#include <omp.h>
                                                                                            float *d a, *d b, *d c;
#endif
                                                         if (a) HPCC free(a);
                                                                                            float scalar;
                                                         if (doIO) {
static int VectorSize;
                                                            fprintf( outFile, "Failed to
                                                                                            cudaMalloc((void**)&d a, sizeof(float)*N);
static double *a, *b, *c;
                                                              allocate memory (%d).\n",
                                                                                            cudaMalloc((void**)&d b, sizeof(float)*N);
                                                             VectorSize );
                                                                                            cudaMalloc((void**)&d c, sizeof(float)*N);
int HPCC StarStream(HPCC Params *params) {
                                                            fclose( outFile );
  int myRank, commSize;
                                                                                            dim3 dimBlock (128);
  int rv, errCount;
                                                                                            dim3 dimGrid(N/dimBlock.x );
                                                         return 1;
  MPI Comm comm = MPI COMM WORLD;
                                                                                            if( N % dimBlock.x != 0 ) dimGrid
  MPI Comm size ( comm, &commSize );
                                                                                            set array<<<dimGrid.dimBlock>>>(d b, .5f, N);
                                                     #ifdef OPENMP
  MPI Comm rank ( comm, &myRank );
                                                                                            set array<<<dimGrid,dimBlock>>>(d c, .5f, N);
                                                     #pragma omp parallel for
                                                                                            scalar=3.0f;
  rv = HPCC Stream( params, 0 == myRank);
                                                       for (j=0; j<VectorSize; j++) {</pre>
                                                                                            STREAM Triad<<<dimGrid,dimBlock>>>(d b, d_c, d_a, scalar, N);
  MPI Reduce ( &rv, &errCount, 1, MPI INT, MPI SUM,
                                                         b[j] = 2.0;
                                                                                            cudaThreadSynchronize();
   0, comm );
                                                         c[i] = 1.0;
                                                                                            cudaFree(d a);
  return errCount;
                                                       scalar = 3.0;
                                                                                            cudaFree (d b);
                                                                                            cudaFree (d c);
                                                     #ifdef OPENMP
int HPCC Stream(HPCC Params *params, int doIO) {
                                                      #pragma omp parallel for
  register int j;
                                                                                            global void set array(float *a, float value, int len) {
                                                     #endif
  double scalar;
                                                                                            int idx = threadIdx.x + blockIdx.x * blockDim.x;
                                                       for (j=0; j<VectorSize; j++)</pre>
                                                                                            if (idx < len) a[idx] = value;
                                                         a[i] = b[i]+scalar*c[i];
  VectorSize = HPCC LocalVectorSize( params, 3,
   sizeof(double), 0);
                                                       HPCC free(c);
                                                                                            global void STREAM Triad( float *a, float *b, float *c,
                                                       HPCC free(b);
  a = HPCC XMALLOC( double, VectorSize );
                                                                                                                        float scalar, int len) {
                                                       HPCC free(a);
 b = HPCC XMALLOC( double, VectorSize );
                                                                                            int idx = threadIdx.x + blockIdx.x * blockDim.x;
  c = HPCC XMALLOC( double, VectorSize );
                                                                                            if (idx < len) c[idx] = a[idx]+scalar*b[idx]; }</pre>
                                                       return 0; }
```

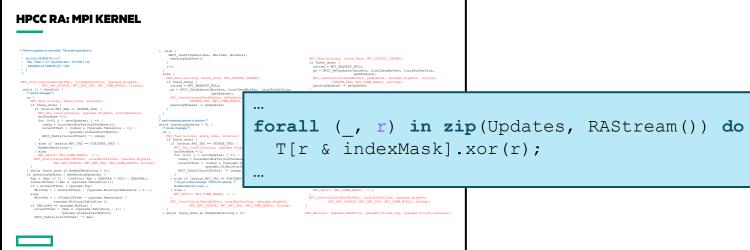
**Note:** This is a trivial parallel computation—imagine the additional complexity for something more realistic...

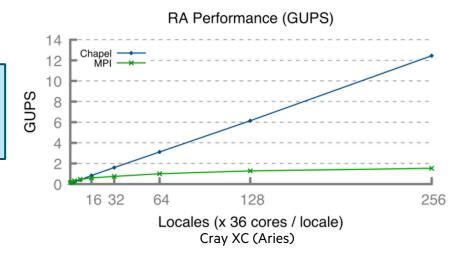
**Challenge:** Can we do better?

# FOR HPC BENCHMARKS, CHAPEL TENDS TO BE CONCISE, CLEAR, AND SCALABLE

```
STREAM TRIAD: C + MPI + OPENMP
                                                                                               use BlockDist:
#include <hpcc.h>
                                                       if (!a || !b || !c) {
  if (c) HPCC free(c);
#ifdef OPENMP
                                                                                               config const m = 1000,
                                                        if (a) HPCC free (a);
                                                          fprintf( outFile, "Failed to allocate memor
static double *a, *b, *c;
                                                          fclose ( outFile );
                                                                                                                                   alpha = 3.0;
int HPCC_StarStream(HPCC_Params *params) {
 int rv, errCount;
                                                                                               const Dom = {1..m} dmapped ...;
                                                     #ifdef OPENMP
                                                      pragma omp parallel for
 MPI_Comm_size( comm, &commSize );
MPI_Comm_rank( comm, &myRank );
                                                       for (j=0; j<VectorSize; j++) {
                                                                                               var A, B, C: [Dom] real;
 rv = HPCC Stream( params, 0 == myRank);
 MPI Reduce ( &rv, &errCount, 1, MPI INT, MPI SUM, 0, comm );
                                                        scalar = 3.0;
 return errCount;
                                                     #ifdef OPENIND
                                                      #pragma omp parallel for
                                                                                               B = 2.0;
int HPCC Stream(HPCC Params *params, int doIO) {
 register int j;
                                                       for (j=0; j<VectorSize; j++)
 double scalar;
                                                                                               C = 1.0;
 VectorSize = HPCC_LocalVectorSize( params, 3, sizeof(double), 0 );
 a = HPCC XMALLOC( double, VectorSize );
                                                       HPCC free(a);
 b = HPCC XMALLOC( double, VectorSize );
 c = HPCC_XMALLOC( double, VectorSize );
                                                       return 0;
                                                                                              A = B + alpha * C;
```



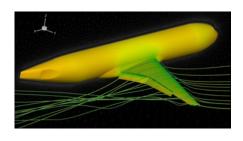




# HOW IS CHAPEL BEING USED IN THE FIELD?

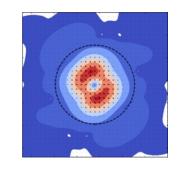


# **CURRENT FLAGSHIP CHAPEL APPLICATIONS**



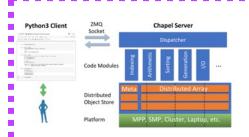
**CHAMPS: 3D Unstructured CFD** 

Éric Laurendeau, Simon Bourgault-Côté, Matthieu Parenteau, et al. École Polytechnique Montréal



# **ChplUltra: Simulating Ultralight Dark Matter**

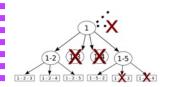
Nikhil Padmanabhan, J. Luna Zagorac, et al. Yale University / University of Auckland



# **Arkouda: NumPy at Massive Scale**

Mike Merrill, Bill Reus, et al.

US DoD



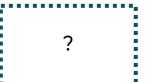
## **ChOp: Chapel-based Optimization**

Tiago Carneiro, Nouredine Melab, et al. INRIA Lille, France



# **CrayAl: Distributed Machine Learning**

Hewlett Packard Enterprise



# Your application here?



# **PARALLEL COMPUTING IN PYTHON?**

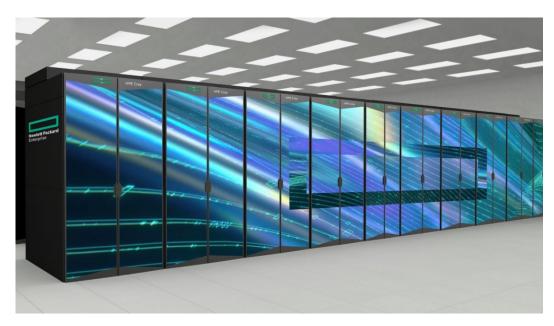
**Motivation:** Say you've got...

...HPC-scale data science problems to solve

...a bunch of Python programmers

...access to HPC systems

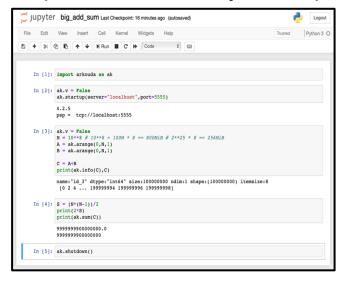




How will you leverage your Python programmers to get your work done?

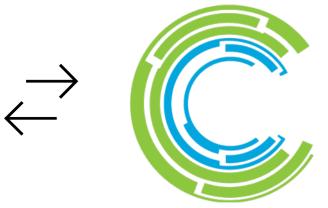
# **ARKOUDA'S HIGH-LEVEL APPROACH**

# Arkouda Client (written in Python)



# **Arkouda Server**

(written in Chapel)









User writes Python code in Jupyter, making NumPy/Pandas calls

# **ARKOUDA SUMMARY**

### What is it?

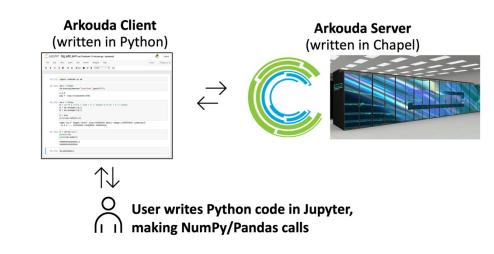
- A Python library supporting a key subset of NumPy and Pandas for Data Science
  - Uses a Python-client/Chapel-server model to get scalability and performance
  - Computes massive-scale results (multi-TB-scale arrays) within the human thought loop (seconds to a few minutes)
- ~20k lines of Chapel, largely written in 2019, continually improved since then

### Who wrote it?

- Mike Merrill, Bill Reus, et al., US DoD
- Open-source: <a href="https://github.com/Bears-R-Us/arkouda">https://github.com/Bears-R-Us/arkouda</a>

# Why Chapel?

- high-level language with performance and scalability
- close to Pythonic
  - enabled writing Arkouda rapidly
  - doesn't repel Python users who look under the hood
- ports from laptop to supercomputer



# **ARKOUDA PERFORMANCE COMPARED TO NUMPY**

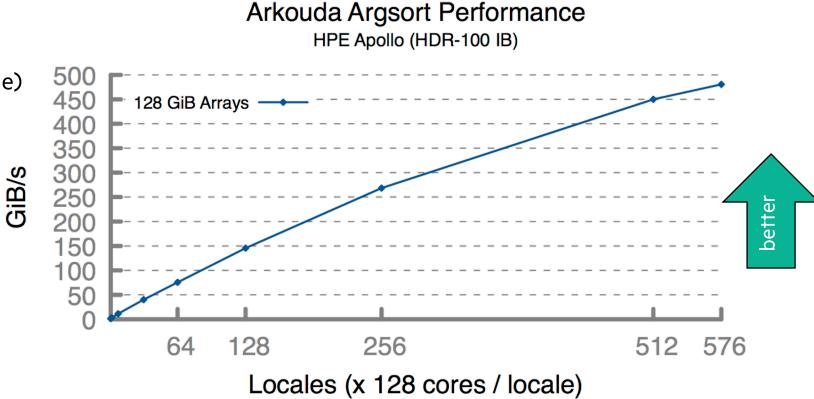
benchmark	NumPy 0.75 GB	Arkouda (serial) 0.75 GB 1 core, 1 node	Arkouda (parallel) 0.75 GB 36 cores x 1 node	Arkouda (distributed) 384 GB 36 cores x 512 nodes
argsort	0.03 GiB/s	0.05 GiB/s	0.50 GiB/s	55.12 GiB/s
		<b>1.66x</b>	<b>16.7</b> x	<b>1837.3x</b>
coargsort	0.03 GiB/s	0.07 GiB/s	0.50 GiB/s	29.54 GiB/s
		<b>2.3x</b>	<b>16.7</b> x	<b>984.7</b> x
gather	1.15 GiB/s	0.45 GiB/s	13.45 GiB/s	539.52 GiB/s
		0.4x	<b>11.7</b> x	<b>469.1</b> x
reduce	9.90 GiB/s	11.66 GiB/s	118.57 GiB/s	43683.00 GiB/s
		<b>1.2</b> x	<b>12.0</b> x	<b>4412.4x</b>
scan	2.78 GiB/s	2.12 GiB/s	8.90 GiB/s	741.14 GiB/s
		0.8x	<b>3.2</b> x	<b>266.6x</b>
scatter	1.17 GiB/s	1.12 GiB/s	13.77 GiB/s	914.67 GiB/s
		1.0x	<b>11.8</b> x	<b>781.8</b> x
stream	3.94 GiB/s	2.92 GiB/s	24.58 GiB/s	6266.22 GiB/s
		0.7x	<b>6.2</b> x	<b>1590.4</b> x

# **ARKOUDA ARGSORT AT MASSIVE SCALES**

• Run on a large Apollo system, summer 2022

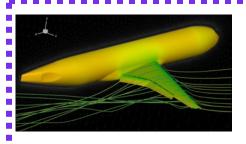
• 73,728 cores of AMD Rome

- 72 TiB of 8-byte values
- 480 GiB/s (2.5 minutes elapsed time)
- ~100 lines of Chapel code



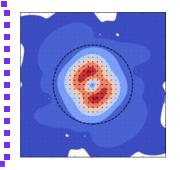
Close to world-record performance—quite likely a record for performance/SLOC

# **CURRENT FLAGSHIP CHAPEL APPLICATIONS**



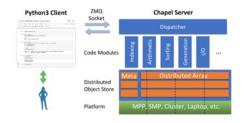
### **CHAMPS: 3D Unstructured CFD**

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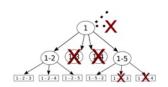
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Hewlett Packard Enterprise

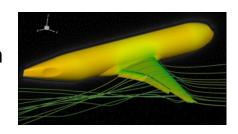
# Your application here?



# **CHAMPS SUMMARY**

### What is it?

- 3D unstructured CFD framework for airplane simulation
- ~100k lines of Chapel written from scratch in ~3 years



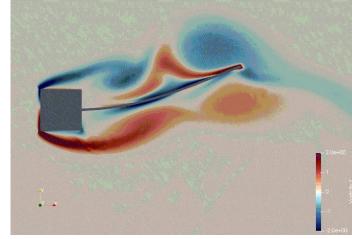
### Who wrote it?

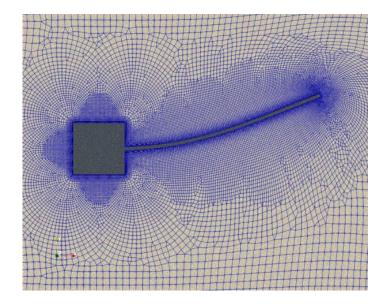
Professor Éric Laurendeau's students + postdocs at Polytechnique Montreal



# Why Chapel?

- performance and scalability competitive with MPI + C++
- students found it far more productive to use







# **CHAMPS: EXCERPT FROM ÉRIC'S CHIUW 2021 KEYNOTE**

# HPC Lessons From 30 Years of Practice in CFD Towards Aircraft Design and Analysis (June 4, 2021)

"To show you what Chapel did in our lab... [our previous framework] ended up 120k lines. And my students said, 'We can't handle it anymore. It's too complex, we lost track of everything.' And today, they went **from 120k lines to 48k lines, so 3x less**.

But the code is not 2D, it's 3D. And it's not structured, it's unstructured, which is way more complex. And it's multi-physics... **So, I've got industrial-type code in 48k lines.**"

"[Chapel] promotes the programming efficiency ... We ask students at the master's degree to do stuff that would take 2 years and they do it in 3 months. So, if you want to take a summer internship and you say, 'program a new turbulence model,' well they manage. And before, it was impossible to do."



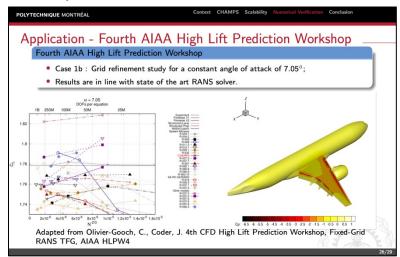


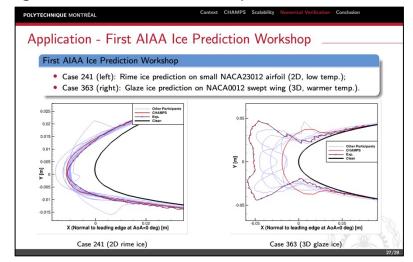
"So, for me, this is like the proof of the benefit of Chapel, plus the smiles I have on my students everyday in the lab because they love Chapel as well. So that's the key, that's the takeaway."

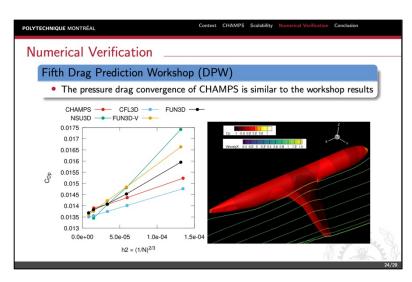
• Talk available online: <a href="https://youtu.be/wD-a\_KyB8al?t=1904">https://youtu.be/wD-a\_KyB8al?t=1904</a> (hyperlink jumps to the section quoted here)

# **CHAMPS HIGHLIGHTS IN 2021**

- Presented at CASI/IASC Aero 21 Conference
- Presented to CFD Society of Canada (CFDSC)
- Participated in 4<sup>th</sup> AIAA High-lift Prediction Workshops, 1<sup>st</sup> AIAA Ice Prediction Workshop
- Reproduced results from 5<sup>th</sup> AIAA Drag Prediction Workshop







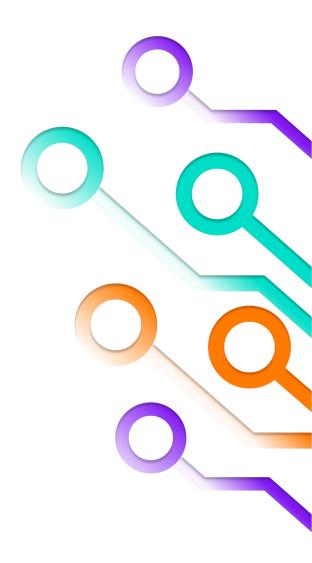
• Generating results comparable to high-profile sites: Boeing, Lockheed Martin, NASA, JAXA, Georgia Tech, ...

# **Looking ahead:**

- giving 6–7 presentations at AIAA Aviation Forum and Exposition, June 2022
- participating in 7<sup>th</sup> AIAA Drag Prediction Workshop



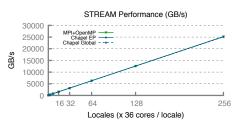
# **WRAPPING UP**



# **SUMMARY**

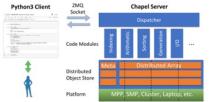
# Chapel is unique among programming languages

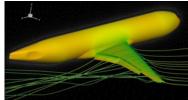
- built-in features for scalable parallel computing make it HPC-ready
- supports clean, concise code relative to conventional approaches
- ports and scales from laptops to supercomputers



# Chapel is being used for productive parallel programming at scale

- users are reaping its benefits in practical, cutting-edge applications
- Arkouda lets Python programmers drive supercomputers from Jupyter





# If you're interested in taking Chapel for a spin, let us know!

• we're happy to work with users and user groups to ease the learning curve





# THE CHAPEL TEAM

Chapel is a team effort—currently made up of 14 full-time employees, 2 part-time, and our director

• we also have 3 more full-time engineers joining in the next few months, and 2 open positions

# **Chapel Development Team at HPE**



see: <a href="https://chapel-lang.org/contributors.html">https://chapel-lang.org/contributors.html</a>
and <a href="https://chapel-lang.org/jobs.html">https://chapel-lang.org/jobs.html</a>

# **CHAPEL RESOURCES**

Chapel homepage: <a href="https://chapel-lang.org">https://chapel-lang.org</a>

(points to all other resources)

### **Social Media:**

• Twitter: <u>@ChapelLanguage</u>

Facebook: @ChapelLanguage

• YouTube: http://www.youtube.com/c/ChapelParallelProgrammingLanguage

# **Community Discussion / Support:**

Discourse: <a href="https://chapel.discourse.group/">https://chapel.discourse.group/</a>

Gitter: <a href="https://gitter.im/chapel-lang/chapel">https://gitter.im/chapel-lang/chapel</a>

• Stack Overflow: <a href="https://stackoverflow.com/questions/tagged/chapel">https://stackoverflow.com/questions/tagged/chapel</a>

GitHub Issues: https://github.com/chapel-lang/chapel/issues



What is Chapel? What's New?

Upcoming Events
Job Opportunities

How Can I Learn Chapel? Contributing to Chapel

Powered by Chapel

**User Resources Developer Resources** 

Social Media / Blog Posts

Presentations
Papers / Publications

Contributors / Credits chapel\_info@cray.com







### The Chapel Parallel Programming Language

### What is Chapel?

Chapel is a programming language designed for productive parallel computing at scale.

Why Chapel? Because it simplifies parallel programming through elegant support for:

- · distributed arrays that can leverage thousands of nodes' memories and cores
- · a global namespace supporting direct access to local or remote variables
- · data parallelism to trivially use the cores of a laptop, cluster, or supercomputer
- task parallelism to create concurrency within a node or across the system

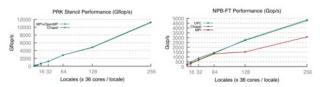
### **Chapel Characteristics**

- · productive: code tends to be similarly readable/writable as Python
- · scalable: runs on laptops, clusters, the cloud, and HPC systems
- · fast: performance competes with or beats C/C++ & MPI & OpenMP
- · portable: compiles and runs in virtually any \*nix environment
- · open-source: hosted on GitHub, permissively licensed

### New to Chapel?

As an introduction to Chapel, you may want to...

- · watch an overview talk or browse its slides
- · read a blog-length or chapter-length introduction to Chapel
- · learn about projects powered by Chapel
- · check out performance highlights like these:



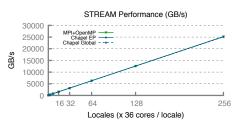
browse sample programs or learn how to write distributed programs like this one:

```
// use the Cyclic distribution library
config const n = 100;
                         // use --n=<val> when executing to override this default
forall i in {1..n} dmapped Cyclic(startIdx=1) do
 writeln("Hello from iteration ", i, " of ", n, " running on node ", here.id);
```

# **SUMMARY**

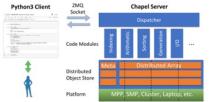
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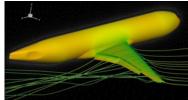
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# **THANK YOU**

https://chapel-lang.org @ChapelLanguage

