Hewlett Packard Enterprise

RAPID PROTOTYPING BY EXAMPLE: ARKOUDA ARGSORT IN CHAPEL

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Rapid Prototyping for Exascale, ECP BoF Days
May 12, 2022

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
  - –Python-like support for rapid prototyping
  - –yet with the performance, scaling, GPU support of Fortran/C/C++, MPI, OpenMP, CUDA, ...

WHAT DO CHAPEL PROGRAMS LOOK LIKE?

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

```
coforall loc in Locales {
  on loc {
    const numTasks = here.maxTaskPar;
    coforall tid in 1..numTasks do
      writef("Hello from task %n of %n on %s\n",
                   tid, numTasks, here.name);
  }
}
```

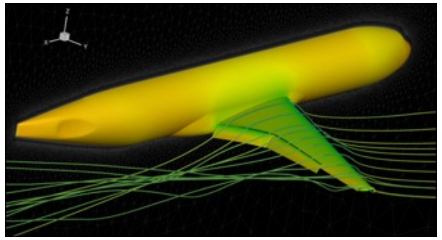
```
> chpl helloTaskPar.chpl
> ./helloTaskPar --numLocales=4
Hello from task 1 of 4 on n1032
Hello from task 4 of 4 on n1032
Hello from task 1 of 4 on n1034
Hello from task 2 of 4 on n1032
Hello from task 1 of 4 on n1033
Hello from task 3 of 4 on n1034
…
```

fillArray.chpl: declare and initialize a distributed array

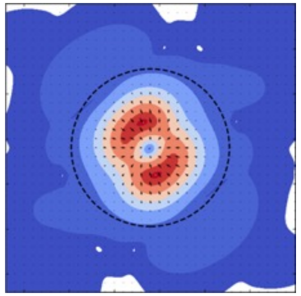
```
use CyclicDist;

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*10 + j + (here.id+1)/10.0;

writeln(A);
```

```
> chpl fillArray.chpl
> ./fillArray --n=5 --numLocales=4
11.1 12.2 13.1 14.2 15.1
21.3 22.4 23.3 24.4 25.3
31.1 32.2 33.1 34.2 35.1
41.3 42.4 43.3 44.4 45.3
51.1 52.2 53.1 54.2 55.1
```

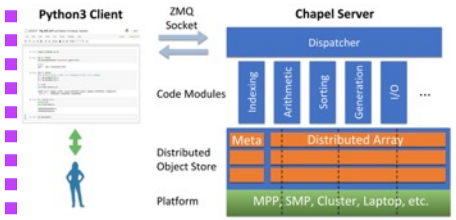
FLAGSHIP CHAPEL APPLICATIONS



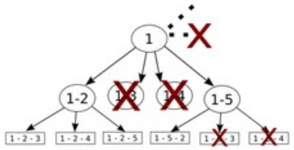
CHAMPS: 3D Unstructured CFD
Éric Laurendeau, Simon Bourgault-Côté, Matthieu Parenteau, et al.
École Polytechnique Montréal



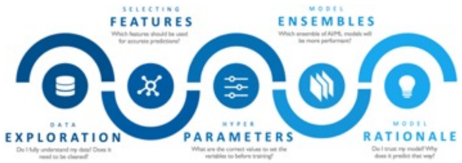
ChplUltra: Simulating Ultralight Dark Matter
Nikhil Padmanabhan, J. Luna Zagorac, *et al.*
Yale University / University of Auckland



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



CrayAI: Distributed Machine Learning
Hewlett Packard Enterprise

?

Your application here?

(images provided by their respective teams and used with permission)

ARKOUDA ARGSORT: PROTOTYPE TO PRODUCTION

Arkouda:

- provides scalable NumPy / Pandas routines for use in data science
- supports massive data sets (multi-TB arrays)
- runs at interactive rates (seconds to a few minutes per operation)
- key, expensive operations: *groupBy* and *argSort*

Arkouda Argsort Milestones:

May 2019: first-draft counting sorts written and tuned

Sept 2019: looked at NESL LSD radix sorts and ~4 hours later had a ~100-line scalable sort

- achieved 80 GiB/s on 512 nodes of Cray XC

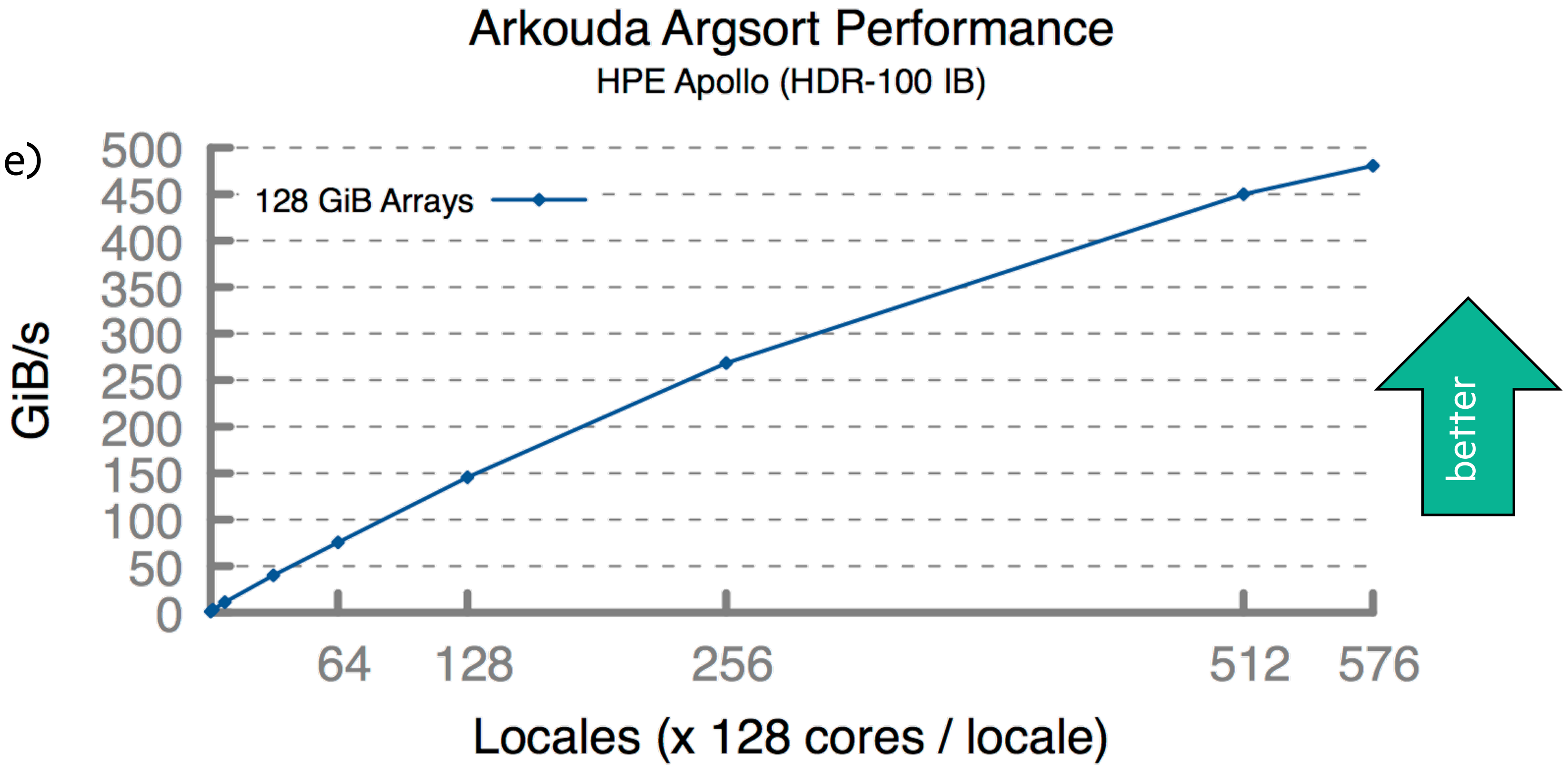
Nov 2019: changed ~12 lines of sort code to aggregate small messages

- 40% improvement on Cray XC, ~1000x improvement on InfiniBand

June 2021: did the following hero run

ARKOUDA ARGSORT AT MASSIVE SCALE

- Ran 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

CHAPEL RESOURCES

Chapel homepage: https://chapel-lang.org

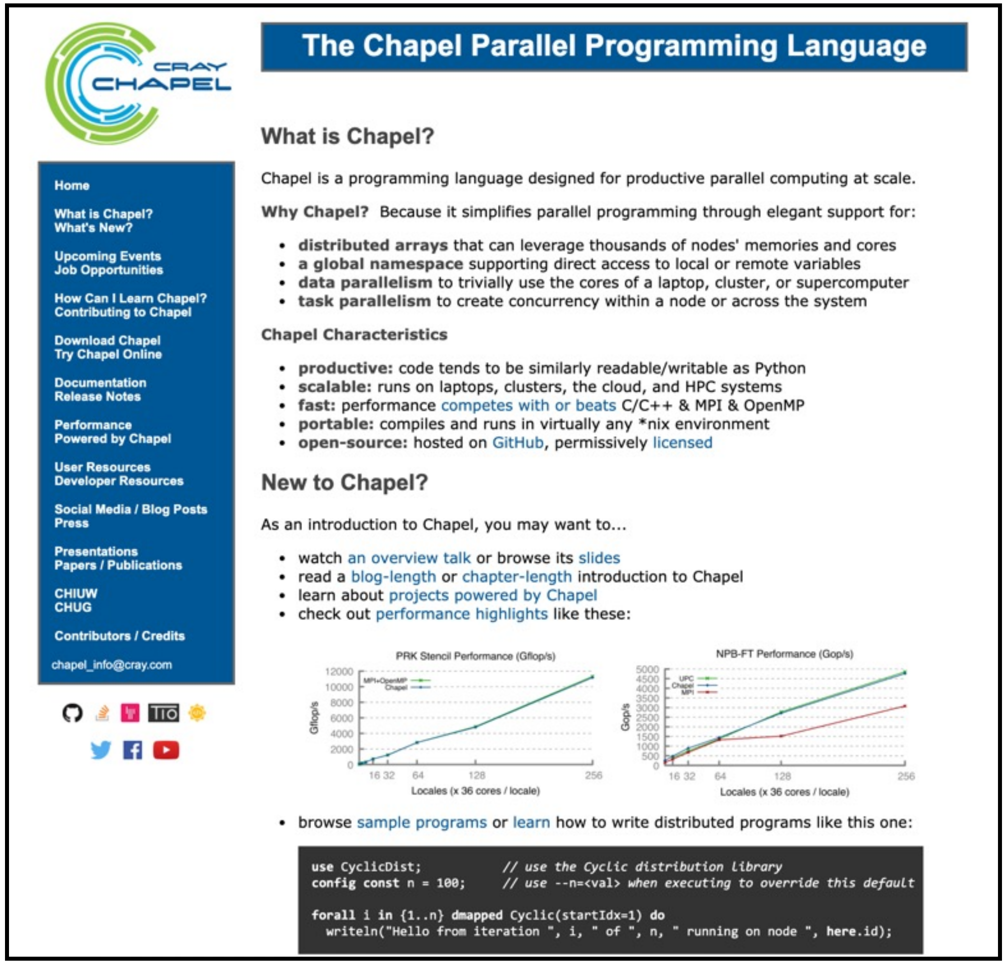
- (points to all other resources)

Social Media:

- Twitter: @ChapelLanguage
- Facebook: @ChapelLanguage
- YouTube: http://www.youtube.com/c/ChapelParallelProgrammingLanguage

Community Discussion / Support:

- Discourse: https://chapel.discourse.group/
- Gitter: https://gitter.im/chapel-lang/chapel
- Stack Overflow: https://stackoverflow.com/questions/tagged/chapel
- GitHub Issues: https://github.com/chapel-lang/chapel/issues



THANK YOU

https://chapel-lang.org
@ChapelLanguage

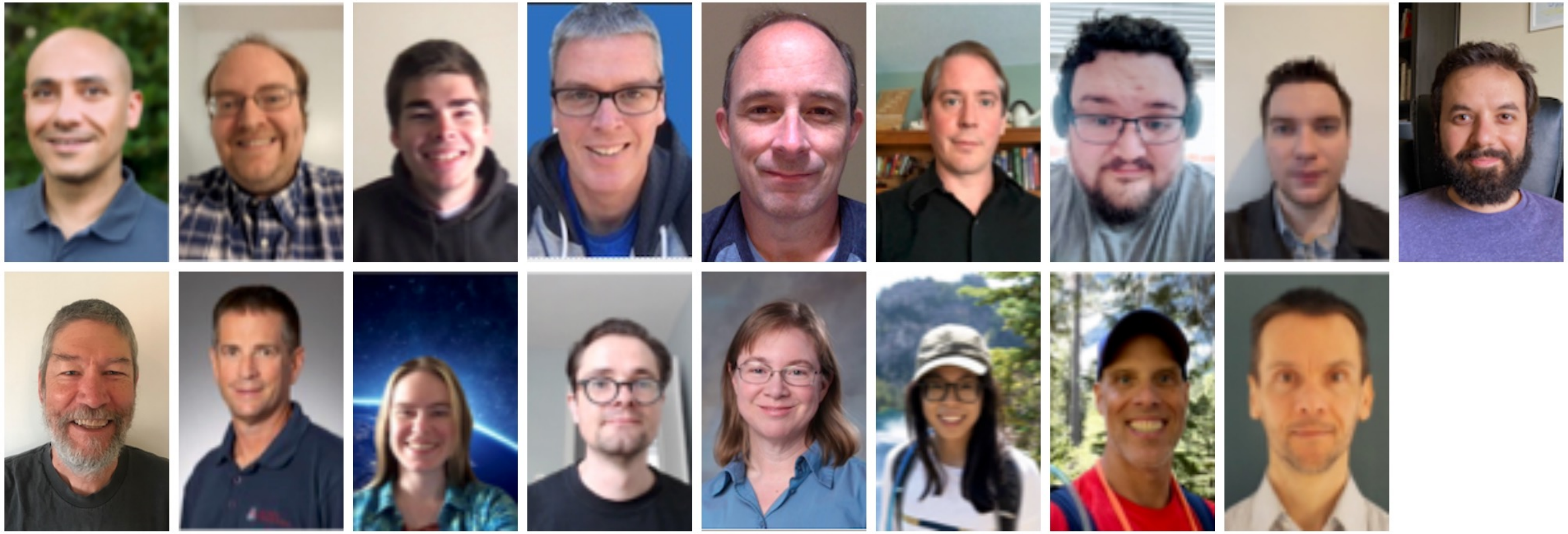
BACKUP SLIDES

THE CHAPEL TEAM

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

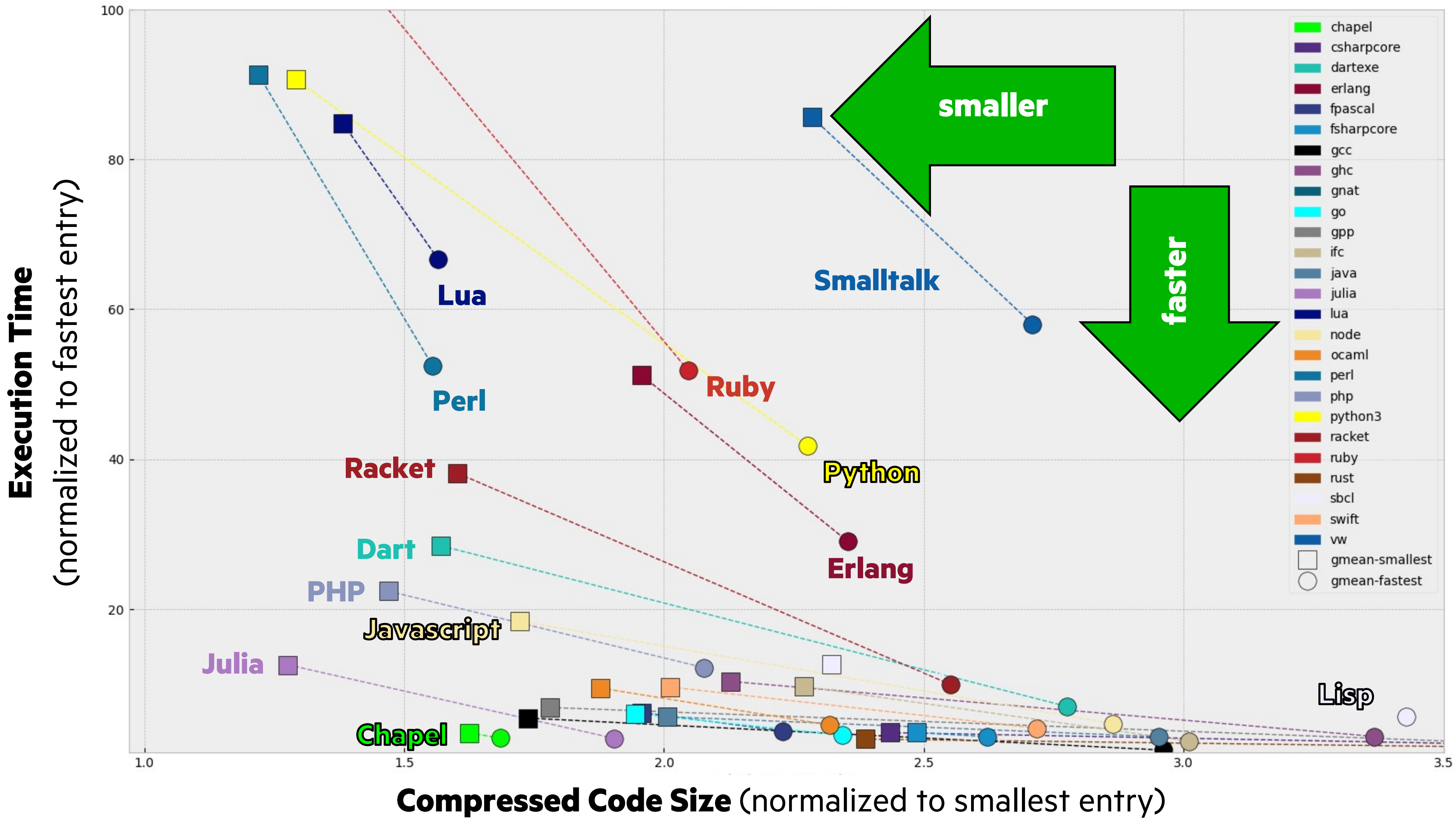
- we also have 3 more full-time engineers joining in the next few months, and 2 open positions

Chapel Development Team at HPE

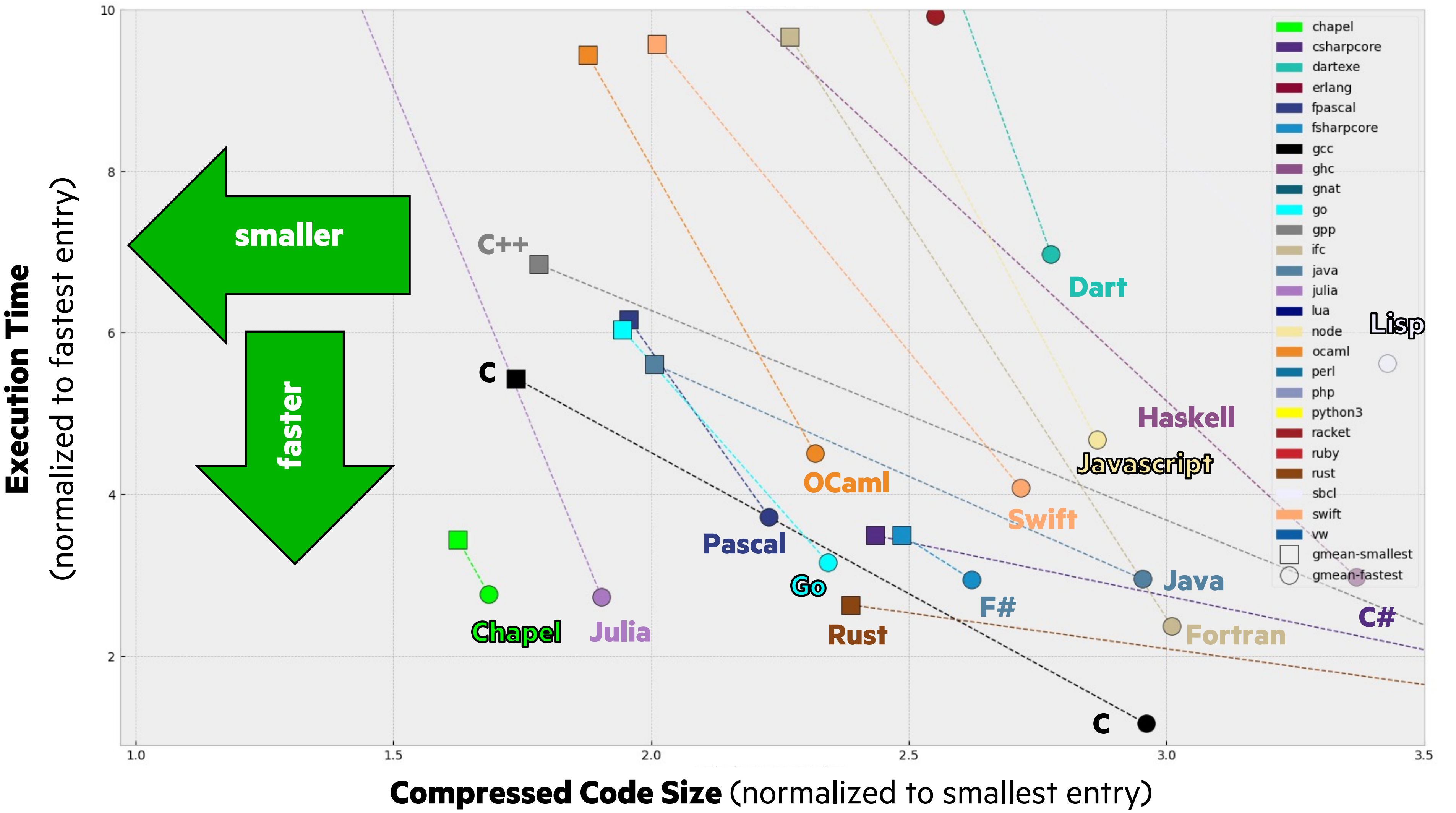


see: https://chapel-lang.org/contributors.html
and https://chapel-lang.org/jobs.html

CLBG: ALL-LANGUAGE SUMMARY (MAY 10, 2022)



CLBG: ALL-LANGUAGE SUMMARY (MAY 10, 2022, ZOOMED-IN)

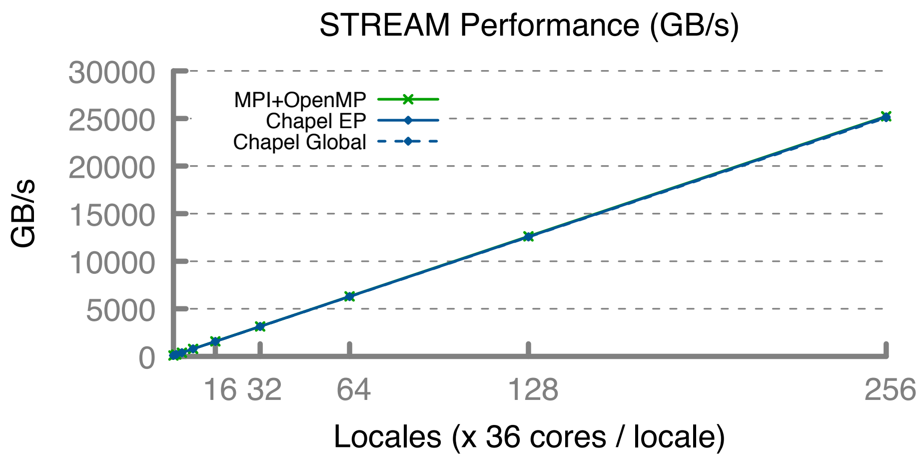


FOR HPC BENCHMARKS, CHAPEL TENDS TO BE CONCISE, CLEAR, AND COMPETITIVE

STREAM TRIAD: C + MPI + OPENMP

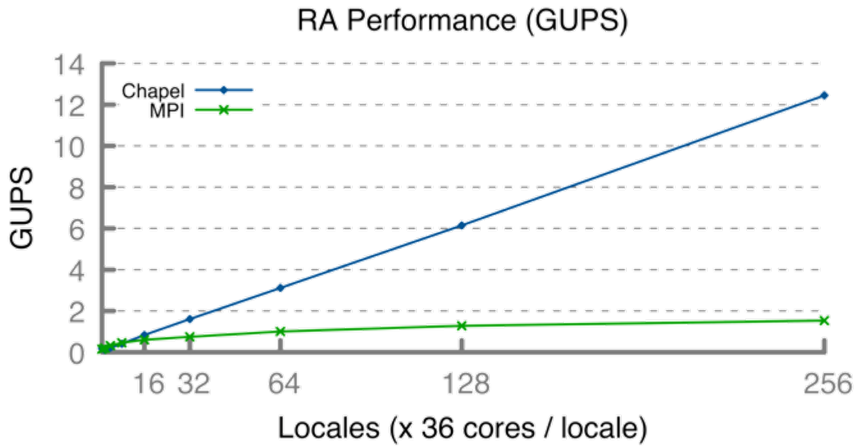
```
#include <hpcc.h>
#ifdef _OPENMP
#include <omp.h>
#endif

static int VectorSize;
static double *a, *b, *c;

int HPCC_StarStream(HPCC_Params *params) {
  int myRank, commSize;
  int rv, errCount;
  MPI_Comm comm = MPI_COMM_WORLD;

  MPI_Comm_size( comm, &commSize );
  MPI_Comm_rank( comm, &myRank );

  rv = HPCC_Stream( params, 0 == myRank);
  MPI_Reduce( &rv, &errCount, 1, MPI_INT, MPI_SUM, 0, comm );

  return errCount;
}

int HPCC_Stream(HPCC_Params *params, int doIO) {
  register int j;
  double  scalar;

  VectorSize = HPCC_LocalVectorSize( params, 3, sizeof(double), 0 );

  a = HPCC_XMALLOC( double, VectorSize );
  b = HPCC_XMALLOC( double, VectorSize );
  c = HPCC_XMALLOC( double, VectorSize );

  if (!a || !b || !c) {
    if (c) HPCC_free(c);
    if (b) HPCC_free(b);
    if (a) HPCC_free(a);
    if (doIO) {
      fprintf( outFile, "Failed to allocate memory
      fclose( outFile );
    }
    return 1;
  }

#ifdef _OPENMP
#pragma omp parallel for
#endif
  for (j=0; j<VectorSize; j++) {
    b[j] = 2.0;
    c[j] = 1.0;
  }
  scalar = 3.0;

#ifdef _OPENMP
#pragma omp parallel for
#endif
  for (j=0; j<VectorSize; j++)
    a[j] = b[j]+scalar*c[j];

  HPCC_free(c);
  HPCC_free(b);
  HPCC_free(a);

  return 0;
}
```

```
use BlockDist;

config const m = 1000,
             alpha = 3.0;
const Dom = {1..m} dmapped …;
var A, B, C: [Dom] real;

B = 2.0;
C = 1.0;

A = B + alpha * C;
```



HPCC RA: MPI KERNEL


```
…
forall (_, r) in zip(Updates, RAStream()) do
  T[r & indexMask].xor(r);
…
```



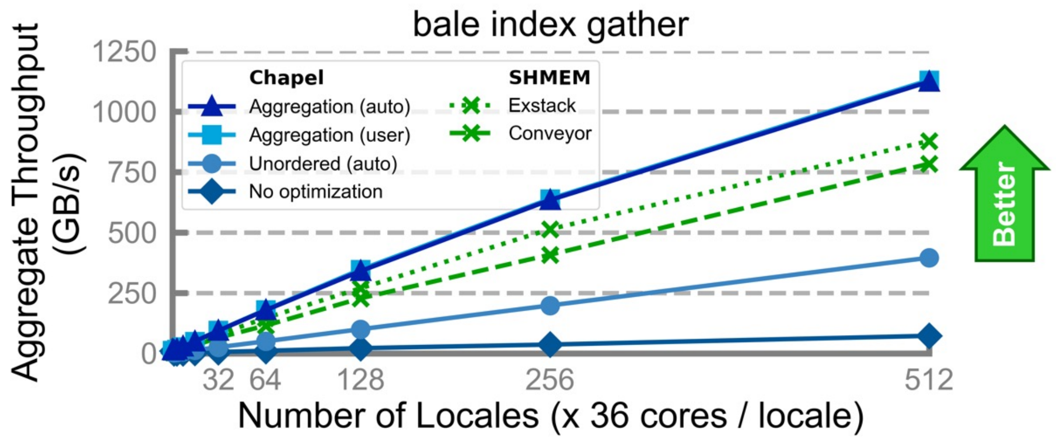
BALE INDEXGATHER

Exstack version

```
i=0;
while( exstack_proceed(ex, (i==l_num_req)) ) {
  i0 = i;
  while(i < l_num_req) {
    l_indx = pckindx[i] >> 16;
    pe   = pckindx[i] & 0xffff;
    if(!exstack_push(ex, &l_indx, pe))
      break;
    i++;
  }

  exstack_exchange(ex);

  while(exstack_pop(ex, &idx , &fromth)) {
    idx  = ltable[idx];
    exstack_push(ex, &idx, fromth);
  }
  lgp_barrier();
  exstack_exchange(ex);

  for(j=i0; j<i; j++) {
    fromth = pckindx[j] & 0xffff;
    exstack_pop_thread(ex, &idx, (uint64_t)fromth);
    tgt[j] = idx;
  }
  lgp_barrier();
}
```

Conveyors version

```
i = 0;
while (more = convey_advance(requests, (i == l_num_req)),
       more | convey_advance(replies, !more)) {

  for (; i < l_num_req; i++) {
    pkg.idx = i;
    pkg.val = pckindx[i] >> 16;
    pe = pckindx[i] & 0xffff;
    if (! convey_push(requests, &pkg, pe))
      break;
  }

  while (convey_pull(requests, ptr, &from) == convey_OK) {
    pkg.idx = ptr->idx;
    pkg.val = ltable[ptr->val];
    if (! convey_push(replies, &pkg, from)) {
      convey_unpull(requests);
      break;
    }
  }

  while (convey_pull(replies, ptr, NULL) == convey_OK)
    tgt[ptr->idx] = ptr->val;
}
```



Cray XC (Aries)

Manually Tuned Chapel version (using aggregator abstraction)

```
forall (d, i) in zip(Dst, Inds) with (var agg = new SrcAggregator(int)) do
  agg.copy(d, Src[i]);
```

Elegant Chapel version (compiler-optimized w/ '--auto-aggregation')

```
forall (d, i) in zip(Dst, Inds) do
  d = Src[i];
```

PARALLEL COMPUTING IN PYTHON?

Motivation: Say you've got…

…HPC-scale data science problems to solve

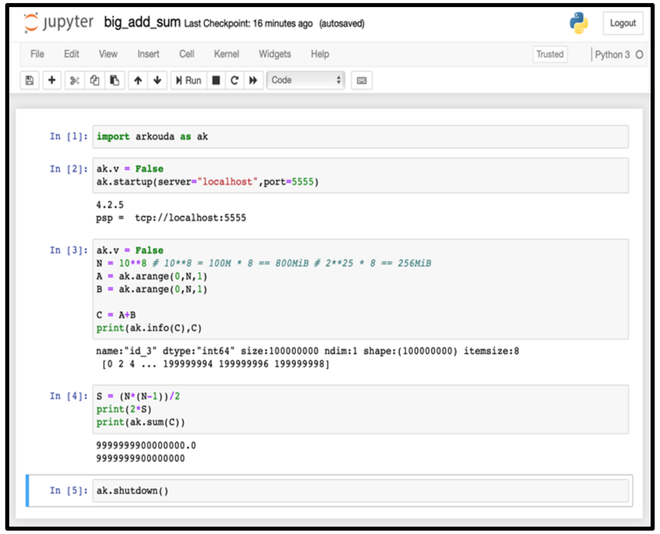
…a bunch of Python programmers

…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

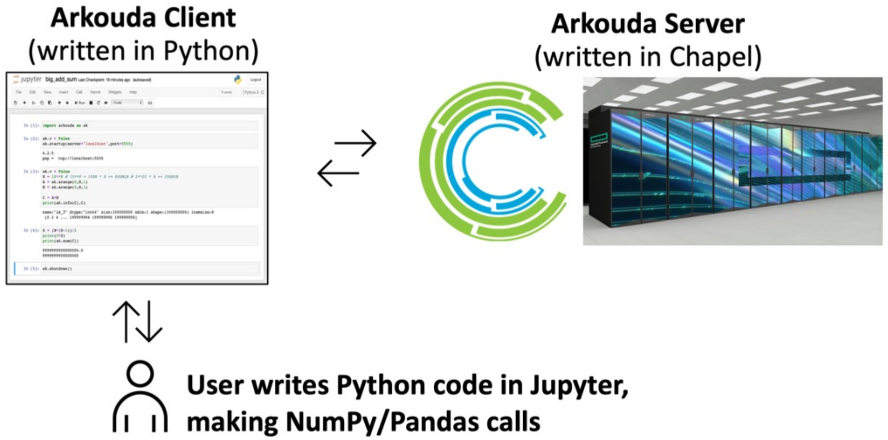
ARKOUDA SUMMARY

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: https://github.com/Bears-R-Us/arkouda



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

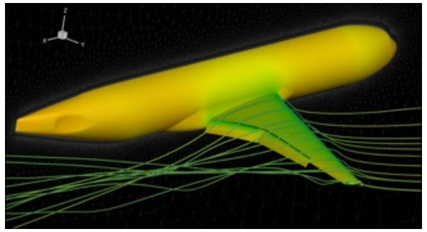
ARKOUDA PERFORMANCE COMPARED TO NUMPY

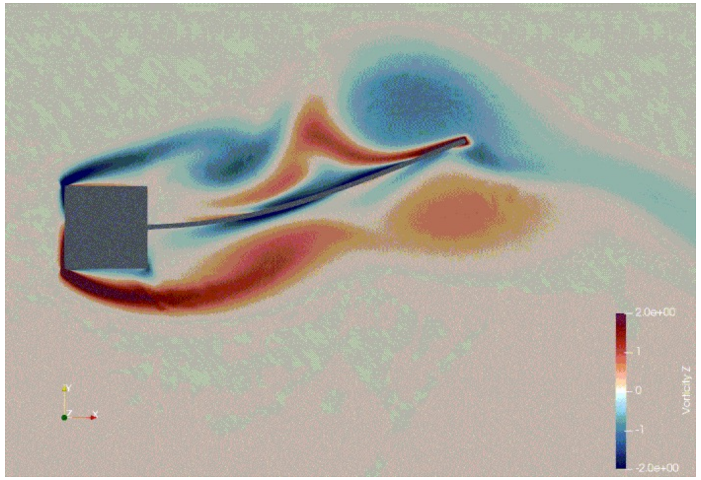
benchmark	NumPy 0.75 GB	Arkouda (serial) 0.75 GB 1 core, 1 node	Arkouda (parallel) 0.75 GB 36 cores x 1 node	Arkouda (distributed) 384 GB 36 cores x 512 nodes
argsort	0.03 GiB/s --	0.05 GiB/s **1.66x**	0.50 GiB/s **16.7x**	55.12 GiB/s **1837.3x**
coargsort	0.03 GiB/s --	0.07 GiB/s **2.3x**	0.50 GiB/s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

CHAMPS SUMMARY

What is it?

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

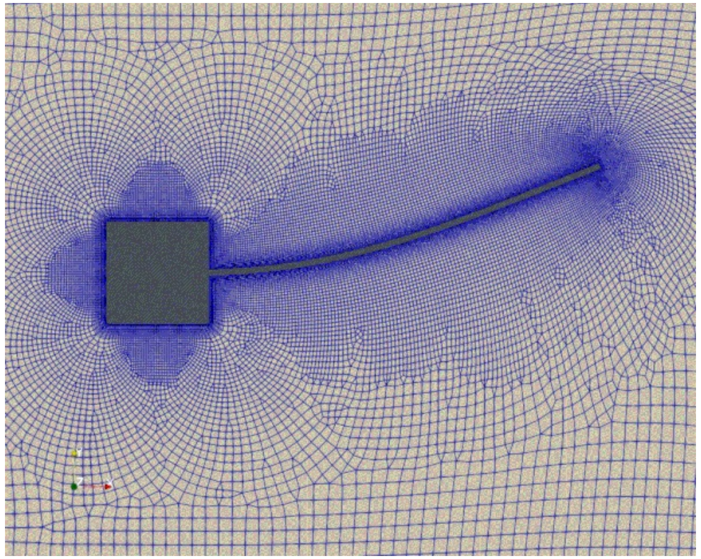




Who wrote it?

- Professor Éric Laurendeau’s students + postdocs at Polytechnique Montreal

POLYTECHNIQUE MONTRÉAL



Why Chapel?

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

(images provided by the CHAMPS team and used with permission)

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."*

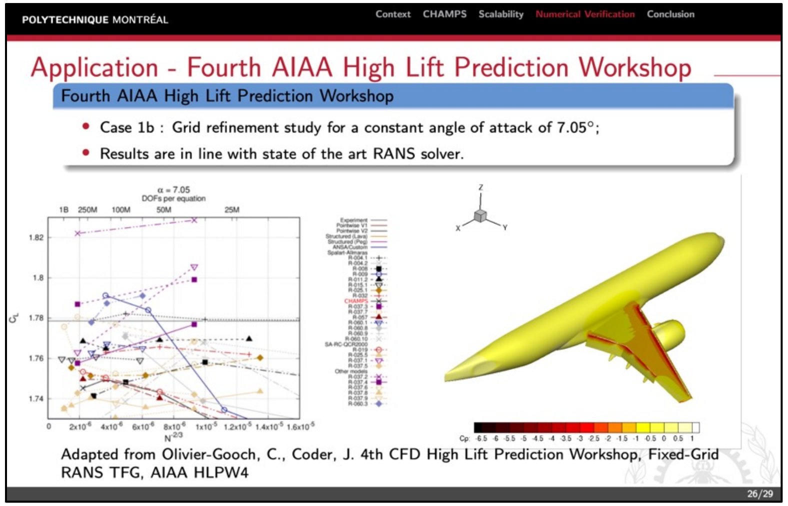
POLYTECHNIQUE MONTRÉAL

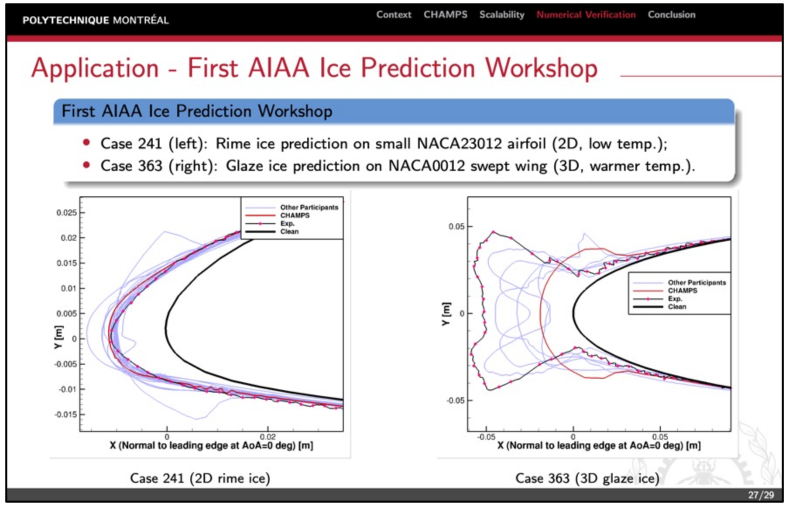
"So, for me, this is like the proof of the benefit of Chapel, ***plus the smiles I have on my students everyday in the lab because they love Chapel as well.*** *So that's the key, that's the takeaway."*

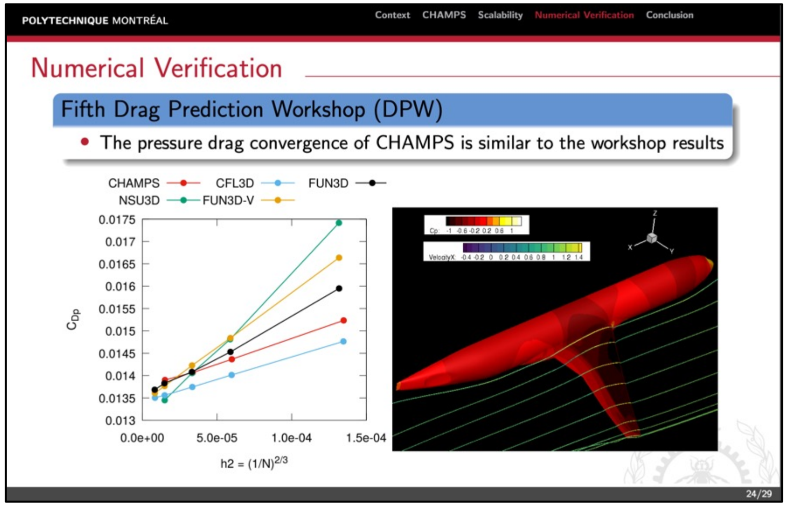
- Talk available online: https://youtu.be/wD-a_KyB8aI?t=1904 (hyperlink jumps to the section quoted here)

CHAMPS HIGHLIGHTS IN 2021

- Presented at CASI/IASC Aero 21 Conference
- Presented to CFD Society of Canada (CFDSC)
- Participated in 4th AIAA High-lift Prediction Workshops, 1st AIAA Ice Prediction Workshop
- Reproduced results from 5th 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 7th AIAA Drag Prediction Workshop

(slide images taken from Éric Laurendeau's SIAM PP22 talk, A Case Study on the Impact of Chapel within an Academic Computational Aerodynamic Laboratory, with permission)