

#### Hewlett Packard Enterprise



# High-Performance, Productive Programming using Chapel with Examples from the CFD Solver CHAMPS

Engin Kayraklioglu, Hewlett Packard Enterprise Éric Laurendeau, Polytechnique Montréal Karim Zayni, Polytechnique Montréal

Advanced Modeling & Simulation (AMS) Seminar Series NASA Ames Research Center, February 20th, 2025

#### **Today's Speakers**



#### Engin Kayraklioglu

Hewlett Packard Enterprise Principal Software Engineer



#### Éric Laurendeau

Polytechnique Montréal Professor



#### Karim Zayni

Polytechnique Montréal Ph.D. Student

### What is Chapel?

### **Chapel: A Modern Parallel Programming Language**

Imagine a programming language for parallel computing that is as... ...**readable and writeable** as Python

...yet also as...

- ...**fast** as Fortran / C / C++
- ...scalable as MPI / SHMEM
- ...GPU-ready as CUDA / HIP / OpenMP / Kokkos ...

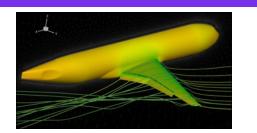
...**portable** as C

...fun as [your favorite programming language]

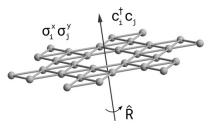


#### This is our motivation for Chapel

### **Applications of Chapel**



**CHAMPS: 3D Unstructured CFD** Laurendeau, Bourgault-Côté, Parenteau, Plante, et al. École Polytechnique Montréal

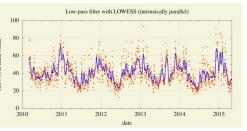


 
 Python3 Client
 ZMQ Socket
 Chapel Server

 Dispatcher
 Dispatcher

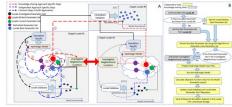
 Dispatcher
 Dispatcher

**Arkouda: Interactive Data Science at Massive Scale** Mike Merrill, Bill Reus, et al. *U.S. DoD* 



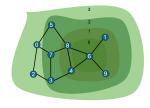
Lattice-Symmetries: a Quantum Many-Body Toolbox Desk dot chpl: Utilities for Environmental Eng.

Tom Westerhout Radboud University

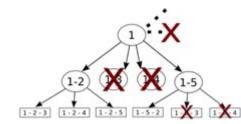


**Chapel-based Hydrological Model Calibration** Marjan Asgari et al. *University of Guelph* 

Nelson Luis Dias The Federal University of Paraná, Brazil



Arachne Graph Analytics Bader, Du, Rodriguez, et al. New Jersey Institute of Technology



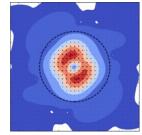
**ChOp: Chapel-based Optimization** T. Carneiro, G. Helbecque, N. Melab, et al. *INRIA, IMEC, et al.* 



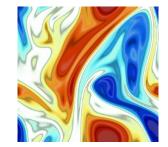
RapidQ: Mapping Coral Biodiversity Rebecca Green, Helen Fox, Scott Bachman, et al. The Coral Reef Alliance



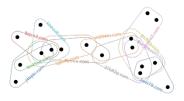
CrayAl HyperParameter Optimization (HPO) Ben Albrecht et al. *Cray Inc. / HPE* 



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



**ChapQG: Layered Quasigeostrophic CFD** Ian Grooms and Scott Bachman University of Colorado, Boulder et al.



**CHGL: Chapel Hypergraph Library** Louis Jenkins, Cliff Joslyn, Jesun Firoz, et al. *PNNL* 

### **Chapel Community**

### **Chapel is Open Source**

chapel Public		🔗 Edit Pins 👻	⊙ Unwatch 64 ▼	😌 Fork 425 👻 📩 Starred 1.8k 👻
° main 👻 양 51 Branches	🛇 <b>48</b> Tags	Go to file t Add fil	e • <> Code •	About
riftEmber Resolve array typ	a Productive Parallel Programming Language			
.github	further limit docs-p	push ghci step	2 weeks ago	𝔅 chapel-lang.org
compiler	make sure tuples of nothing are properly removed 5 days ago			language programming-language
doc	clarify build require	clarify build requirements last week		
frontend	Resolve array type	es with module code in dyno (#26628)	6 hours ago	parallel-computing distributed-computing scientific-computing
highlight	add missing keywo	ords to chpl-mode.el	4 months ago	high-performance-computing chapel
make	Extend clang 18 de	eprecation warning silencing to 19	2 weeks ago	productive

github.com/chapel-lang/chapel

### **Community Events**

- Office hours, live coding sessions, teaching meetups, language design discussions (new!)
- Annual conference ChapelCon

chapel-lang.org/community/

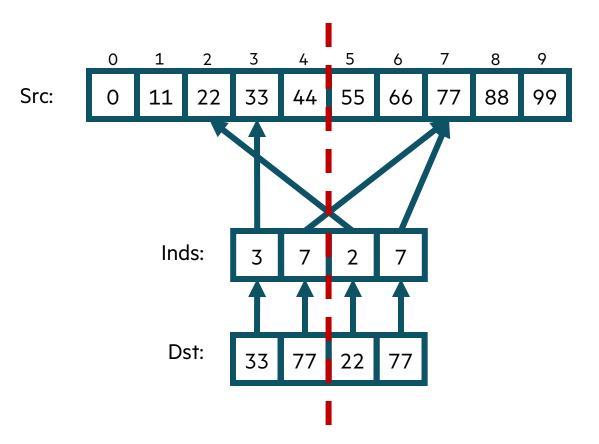
### Chapel is joining the High Performance Software Foundation





### What does Chapel code look like?

#### Bale IndexGather (IG): In Pictures



#### **Bale IG in Chapel: Array Declarations**

config const n = 10, 0 1 2 3 4 5 6 7 89 m = 4;Src: Inds: var Src: [0..<n] int,</pre> Inds, Dst: [0..<m] int;</pre> Dst: Ş

#### **Bale IG in Chapel: Compiling**

config const n = 10, 0 1 2 3 4 5 6 7 89 m = 4;Src: Inds: var Src: [0..<n] int,</pre> Inds, Dst: [0..<m] int;</pre> Dst:



#### **Bale IG in Chapel: Executing**



Inds:	
-------	--





#### Bale IG in Chapel: Executing, Overriding Configs

config const n = 10, m = 4;

var Src: [0..<n] int, Inds, Dst: [0..<m] int;</pre>

```
$ chpl bale-ig.chpl
$ ./bale-ig --n=1_000_000 --m=1_000_000
$
```

### **Bale IG in Chapel: Array Initialization**

<b>use</b> Random;	
<pre>config const n = 10, m = 4;</pre>	0       1       2       3       4       5       6       7       8       9         Src:       0       11       22       33       44       55       66       77       88       99
<pre>var Src: [0<n] int,<br="">Inds, Dst: [0<m] int;<="" pre=""></m]></n]></pre>	Inds: 3 7 2 7
<pre>Src = [i in 0<n] fillrandom(inds,="" i*11;="" max="n-1);&lt;/pre" min="0,"></n]></pre>	Dst:
<pre>\$ chpl bale-ig.chpl</pre>	

\$ ./bale-ig

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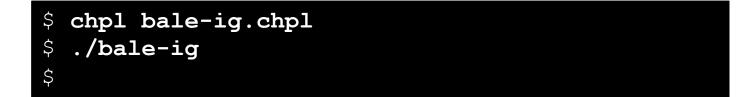
#### **Bale IG in Chapel: Serial Version**

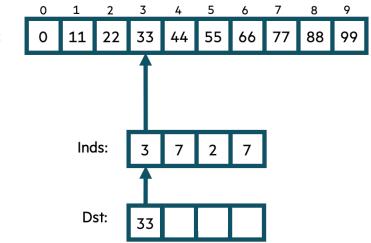
config const n = 10, 1 2 3 4 5 6 7 8 9 0 m = 4;Src: 0 11 22 33 44 55 66 77 88 99 Inds: var Src: [0..<n] int,</pre> 3 7 2 Inds, Dst: [0..<m] int;</pre> ... Dst: 33 for i in 0..<m do Dst[i] = Src[Inds[i]];

\$ chpl bale-ig.chpl
\$ ./bale-ig
\$

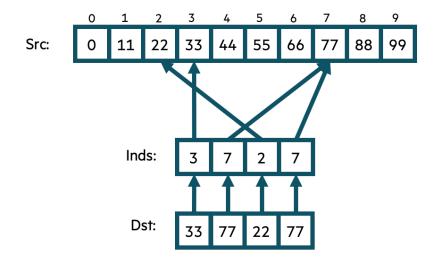
#### **Bale IG in Chapel: Serial, Zippered Version**

config const n = 10, m = 4; var Src: [0..<n] int, Inds, Dst: [0..<m] int; ... for (d, i) in zip(Dst, Inds) do d = Src[i];



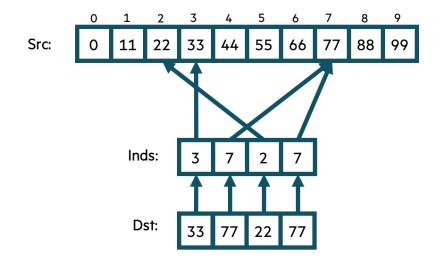


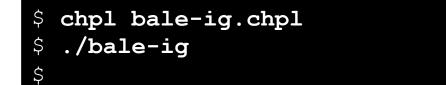
```
config const n = 10,
    m = 4;
var Src: [0..<n] int,
    Inds, Dst: [0..<m] int;
...
foreach (d, i) in zip(Dst, Inds) do
    d = Src[i];
```

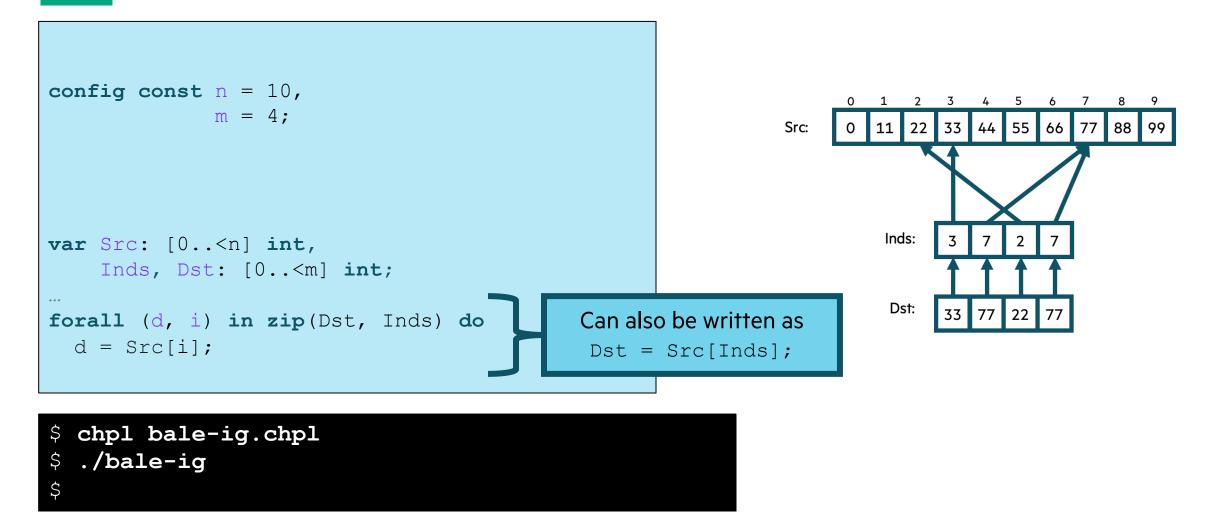


\$ chpl bale-ig.chpl
\$ ./bale-ig
\$

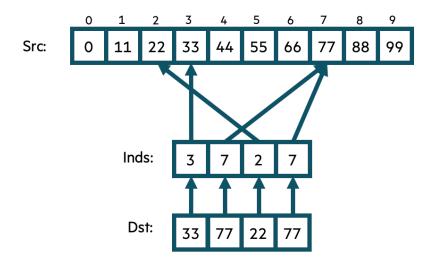
```
config const n = 10,
    m = 4;
var Src: [0..<n] int,
    Inds, Dst: [0..<m] int;
...
forall (d, i) in zip(Dst, Inds) do
    d = Src[i];
```







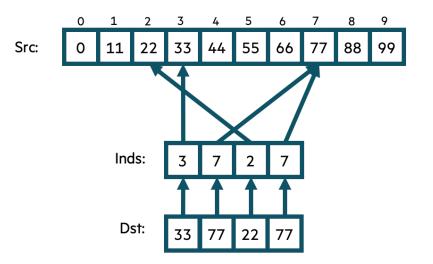
```
config const n = 10,
    m = 4;
var Src: [0..<n] int,
    Inds, Dst: [0..<m] int;
...
forall (d, i) in zip(Dst, Inds) do
    d = Src[i];
```



\$ chpl bale-ig.chpl
\$ ./bale-ig
\$

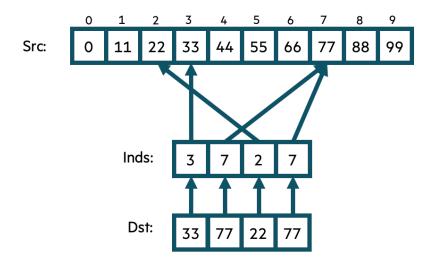
#### **Bale IG in Chapel: Parallel, Zippered Version for a GPU**

```
config const n = 10,
    m = 4;
on here.gpus[0] {
  var Src: [0..<n] int,
    Inds, Dst: [0..<m] int;
...
forall (d, i) in zip(Dst, Inds) do
    d = Src[i];
}
```





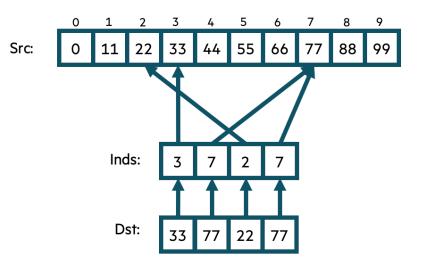
```
config const n = 10,
    m = 4;
var Src: [0..<n] int,
    Inds, Dst: [0..<m] int;
...
forall (d, i) in zip(Dst, Inds) do
    d = Src[i];
```



\$ chpl bale-ig.chpl
\$ ./bale-ig
\$

### Bale IG in Chapel: Parallel , Zippered Version with Named Domains (Multicore)

```
config const n = 10,
    m = 4;
const SrcInds = {0..<n},
    DstInds = {0..<m};
var Src: [SrcInds] int,
    Inds, Dst: [DstInds] int;
...
forall (d, i) in zip(Dst, Inds) do
    d = Src[i];
```

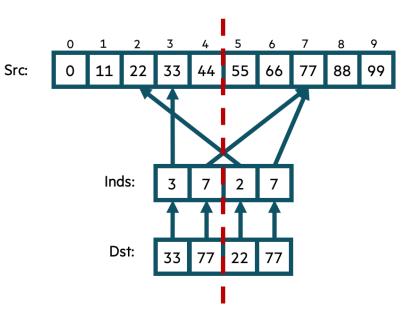




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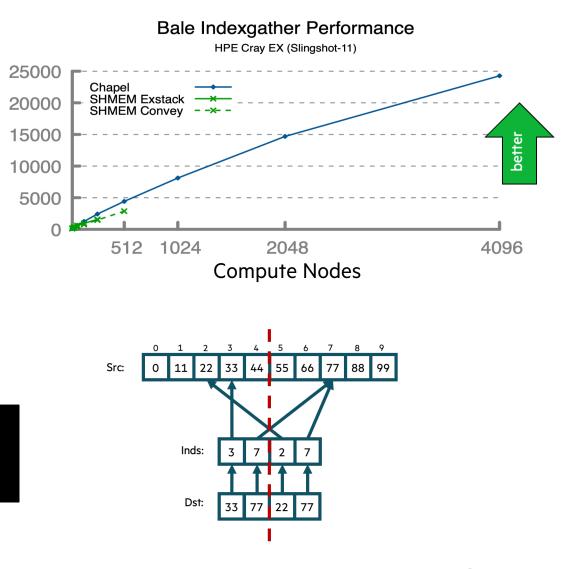
#### **Bale IG in Chapel: Distributed Parallel Version**





### **Bale IG in Chapel: Distributed Parallel Version**

```
use BlockDist;
config const n = 10,
             m = 4;
                                                     GB/s
const SrcInds = blockDist.createDomain(0..<n),</pre>
      DstInds = blockDist.createDomain(0..<m);</pre>
var Src: [SrcInds] int,
    Inds, Dst: [DstInds] int;
...
forall (d, i) in zip(Dst, Inds) do
  d = Src[i];
  chpl bale-ig.chpl --fast --auto-aggregation
Ş
  ./bale-ig -nl 4096
Ş
$
```



### **CHAMPS: CHApel Multi-Physics Software**

## Computational Aerodynamics R&D efforts within Academia

Vision for transonic aerodynamic modeling

- CFD via RANS has matured and is fully integrated within industrial workflows
  - o Including adjoint-based optimization
  - o Full-flight envelope remains elusive (e.g. unsteady flows)
- CFD's integration within multidisciplinary applications has yet to reach maturity
  - $\circ$   $\;$  Static-Aeroelasticity, including adjoint, has been thoroughly studied
  - $\circ$   $\$  More holistic problems can only be achieved with multi-fidelity approach

MDO Level	Fidelity	Aerodynamics	Structures	Propulsion			
CMDO	LO	Knowledge-based aerodynamics	Knowledge-based weight prediction	Fixed architecture, scaled engine model			
	L1	Quasi-3D methods (3D VLM / Panel method + 2D High-Fidelity CFD)	Beam or thin-shell models	Variable architecture, generic rubber engine			
	L1.5	Disciplinary L2 Surrogate Models		Surrogate model(s) from Engine supplier(s)			
PMDO	L2	Mid-to-High Fidelity CFD (3D TSD to RANS)	Global FEM				
	L2.5	Disciplinary L3 Surrogate Models		Real engine model (fixed)			
	L3	RANS	Detail FEM				

#### Table 1 MDO levels and tool sets

#### Source:

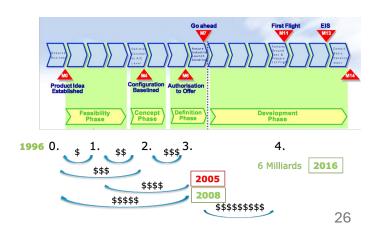
Piperni et al., Development of a Multilevel Multidisciplinary-Optimization Capability for an Industrial Environment, AIAA J, 2013.

#### • Case study: C-Series/A220

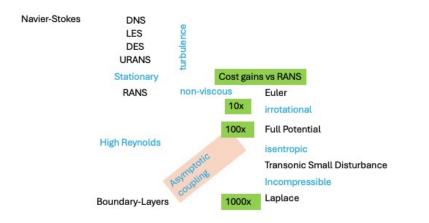
Sources:

Flaig, Axel. Airbus 380: Solutions to the aerodynamic Challenges of Designing the World's Largest Passenger Aircraft, 2008

Wikipedia for cost+years

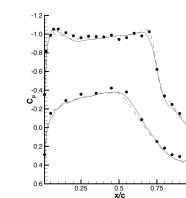


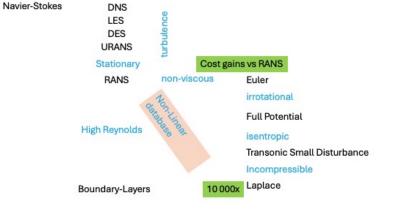
## Aerodynamic modeling choices



#### Boundary-Layer Coupling Schemes

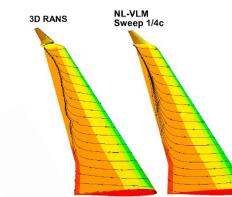
Captures shock-waves + flow separation





#### High Fidelity Database

Allows easy AI/ML treatment



Boudreau, J. & Laurendeau, E., drag Prediction Using the Euler/Navier-Stokes Code FANSC, SAE 2003-01-3022

> Parenteau et al., VLM Coupled with 2.5D RANS Sectional Data for High-Lift Design, AIAA 2018-1049

## Academic Research Constraints

- Very High Turnaround of High-Quality Personnel (HQP)
  - Undergrad Summer Research (0.3 years), MSc (2 years), PhD (3-4 years), Post-Docs (2-years)
- Industrial Research Contracts and needs for 3D Full Aircraft Aerodynamic Modeling
  - Master complete workflow: geometry, mesh generation, flow solver, post-processing
  - o Acquire multi-disciplinary and multi-fidelity knowledge
- High-Performance Computing 'barrier'
  - Complex Source Codes, despite great advances in computer sciences
  - Computational efficiency, a nice-to-have is now a must-have to perform analysis or optimization
  - OPEN-MP + MPI paradigms makes for O(Million) lines of code

## Academic Laboratory Solutions

#### • Cascading complexity stream of problems

- Fundamental to applied problems
- MSc (2D, single disciplinary), PhD (3D, multidisciplinary), Post-doc (high TRL levels)

#### Large laboratory

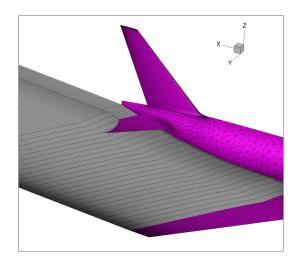
- Flat governance structure
- Collaboration with single-disciplinary specialists (e.g. optimization, AI, etc.)
- o International collaboration, great also for training HQP
- High-Performance Computing
  - New unstructured RANS-based software using Chapel language: CHAMPS

## CHAMPS: Advanced 2D-3D CFD Solver

#### **Overview of CHAMPS (Chapel Multi-Physics Software)**

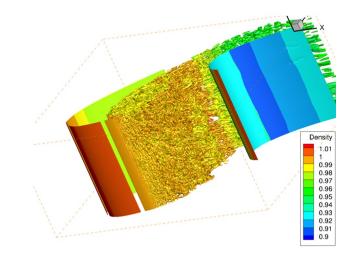
- Cutting-edge Computational Fluid Dynamics (CFD) solver
- 2D and 3D simulations using unstructured meshes.
- Three levels of fidelity for complex aerodynamic and multi-physics problems.
- Solves the Reynolds-Averaged Navier-Stokes (RANS) equations using second-order finite volume methods.
- Supports advanced convective flux schemes like Roe and AUSM.
- Includes Spalart-Allmaras (SA), k-ω SST-V, and Langtry-Menter transition models.
- Explicit Runge-Kutta solver, Implicit solvers including SGS and GMRES for enhanced stability.
- Linked with external libraries such as MKL, CGNS, METIS, MMG, CGAL and PETSc.
- Simulates icing phenomena using both deterministic and stochastic approaches.
- Handles fluid-structure interactions for advanced aerodynamics studies.

### CHAMPS: Multi-Fidelity Transonic Viscous Flows



Medium Fidelity ~O(mins):

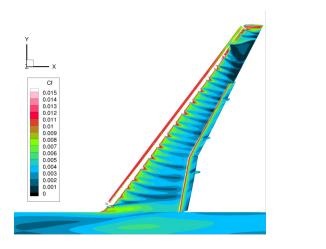
- Euler (Coupling with Boundary Layer)
- Non Linear Vortex Lattice Method (NL-VLM)

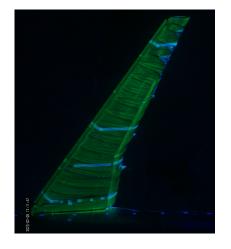


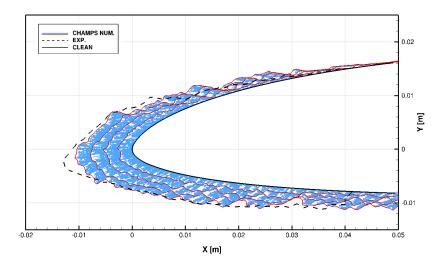
High Fidelity ~O(Hours/Days):

- Unsteady Reynolds Averaged Navier Stokes (U-RANS)
- Wall Model Large Eddy Simulation (WMLES)
- Detached Eddy Simulation (DES)

## CHAMPS: Expertise & Global Impact







- Current Development team consists of 6 PhD and 3 MSc students
- Used at Université Strasbourg (France), Prof. Hoarau
- Used in Polytechnique Montréal's graduate class in Computational Aerodynamics
- CHAMPS has contributed to over 50 publications, including 10 journal articles
- Workshops Participation:
  - High Lift Prediction Workshops (HLPW): 4 and 5th Editions
  - Drag Prediction Workshops (DPW): 6, 7 and 8th Editions
  - Ice Prediction Workshops (IPW) : 1st and 2nd Editions

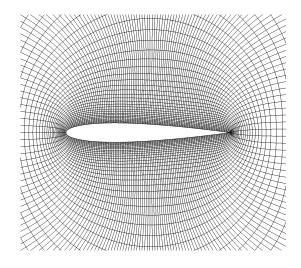
## CHAMPS: Advanced 2D-3D CFD Solver

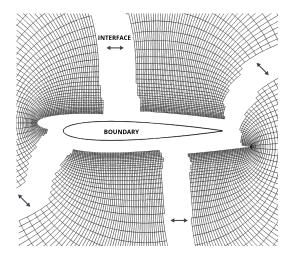
#### **Codebase Statistics:**

- CHAMPS : ~150K lines of code
- **Pre-Processor**: ~17K lines
- Flow Solver: ~15K lines
- Turbulence Solver: ~13K lines
- Droplet Solver (Eulerian + Lagrangian): ~24K lines
- **Post-Processor**: ~2K lines
- Smaller Solvers: ~5K lines (each)
- Shared Structure & APIs : ~50K lines

## Parallel CFD for HPC

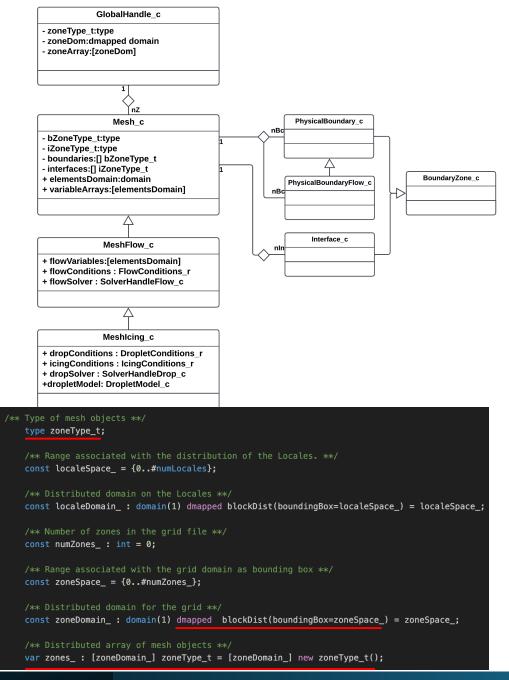
- Volumetric Meshing around complex geometries
- 2D Meshes : Ranging from 0.5 to 1.0 Million Unknowns
- 3D Meshes : Handling up to 1 Billion Unknowns
- Leveraging HPC to significantly reduce computation time
- Problem is partitioned into smaller sub-problems interconnected via interfaces
- Each sub-problem runs independently on dedicated tasks
- Minimizing communication overhead to maximize overall efficiency





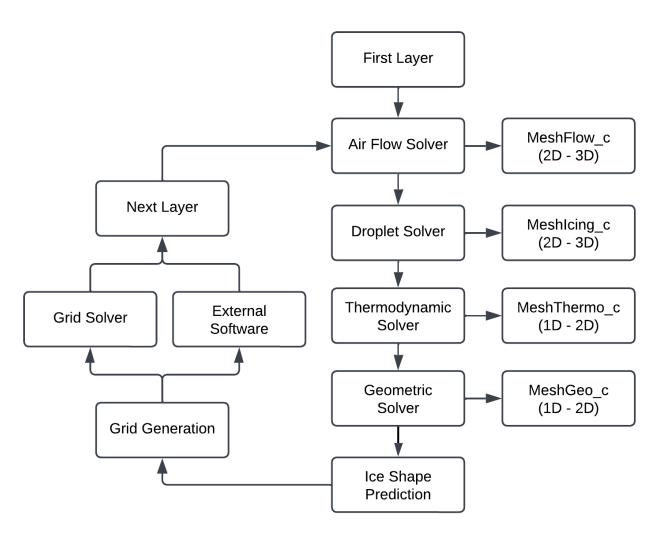
### Software Structure : Framework

- Multiphysics problems require different computational domains grid (*Mesh\_c*)
- *Type* aliases in *Chapel* are used to define computational domains at the start of each simulations
- Supports Generic Programming and Improve flexibility
- Distributed *domains* enable efficient handling of large-scale simulations across multiple computational nodes



## Software Structure : Icing Framework

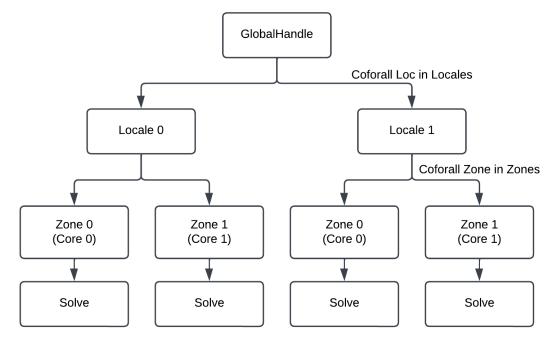
- Typical icing simulations involve four distinct computational domains
- Some domains solve the volume field (3D), while others focus on surface interactions (2D)
- Each computational domain has its own specific characteristics, variables and requirements



## Software Structure :

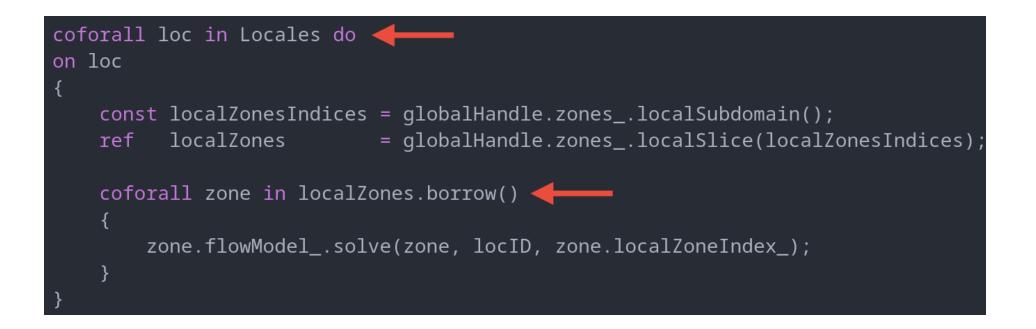
**Top-level Overview** 

- Each simulation runs in a single execution (using a *GlobalHandle*), ensuring efficiency and consistency.
- Tasks are distributed hierarchically using *coforall* statements, first at the Locale (node) level, then further subdivided at the Zone (core) level to maximize parallelism.
- Grid partitioning through METIS guarantees optimal load balancing across all cores, enhancing computational efficiency and minimizing idle time.



```
proc main(args : [] string)
{
    // Fetching user inputs for the flow
    var flowInputs : FlowInputs_r;
    var turbInputs : TurbInputs_r;
    ref commonInputs = flowInputs.commonInputs_;
    var globalHandle : GlobalHandleFlow_t = initializeComputationalDomain(GlobalHandleFlow_t, commonInputs);
    try! writeln("Elapsed time after reading grid: ", clock.elapsed());
    runFlowSimulation(globalHandle.borrow(), clock, flowInputs, turbInputs);
}
```

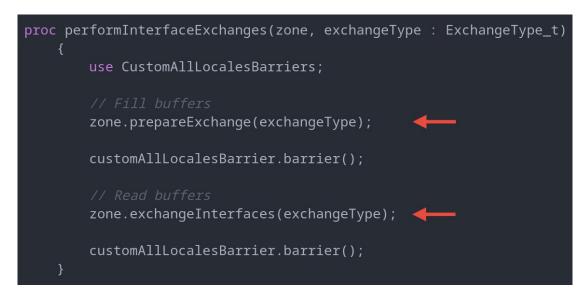
- Type GlobalHandleFlow\_t will initialize MeshFlow\_t computational domains
- One proc to run : runFlowSimulation()

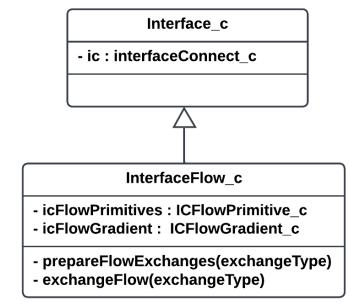


- First coforall will loop over Locales
- Second *coforall* will loop over cores to execute Solve()
- Provides greater control of each computational domain's operations

## Software Structure : Data Exchanges

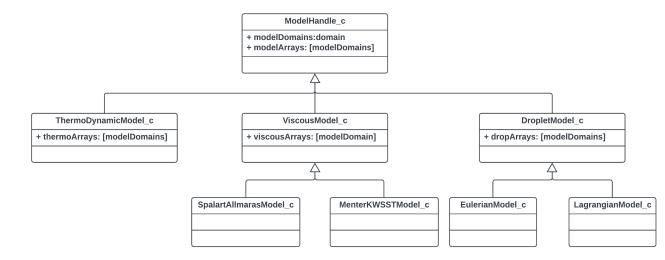
- Each *interface* is equipped with an *interfaceConnect* to facilitate seamless communication with adjacent zones.
- Each zone prepares for data exchanges by populating its respective buffer arrays, ensuring that all necessary information is readily available for transfer.
- Custom synchronization barriers are implemented to maximize efficiency.
- Once synchronization is achieved, all data exchanges are executed simultaneously, minimizing communication overhead and maximizing throughput.
- The global namespace support provided by *Chapel* ensures that any task can access the necessary buffers, regardless of its location across Locales.





## Software Structure : Generics & Modularity

- All models inherit from a base ModelHandle\_c Class
- Maximize code reusability, leading to faster implementation and enhance readability
- *Where* statements are needed to prevent compilation errors.
- This ensures compatibility when fields or methods are not present in the parent class.
- *Where* statements also prevent conflicts with sibling classes (other children of the same parent).



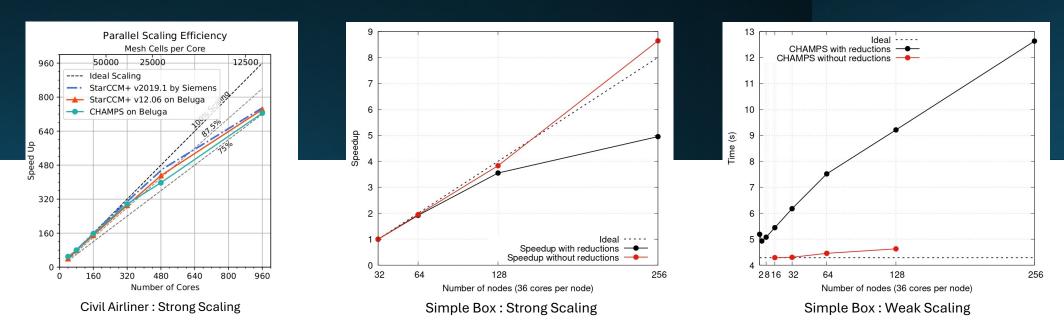
override proc solve(zone, locId : int, localTaskID : int)
where isProperSubtype(zone.type, MeshThermo\_c)

## Software Structure : Model Implementation

- Viscous models are decided based on user input at the start of runFlowSimulation()
- Leads to the instantiation of a new viscousModel\_c object in each zone

```
proc initializeViscousModelAndSolver(globalHandle, zone, flowInputs : FlowInputs_r, turbInputs : TurbInputs_r,
    select flowInputs.FLOW_REGIME_
        when FlowRegime_t.INVISCID
           zone.viscousModel_ = new owned InviscidModel_c();
        when FlowRegime_t.LAMINAR
           zone.viscousModel_ = new owned LaminarModel_c();
        when FlowRegime_t.TURBULENT
           select turbInputs.TURB_MODEL_
               when TurbulenceModel_t.SA
                   zone.viscousModel_ = new owned SpalartAllmarasModel_c(zone, turbInputs);
               when TurbulenceModel_t.KW
                   zone.viscousModel_ = new owned MenterKWSSTModel_c(zone, turbInputs);
           zone.viscousModel_.initializeConditionsAndSolvers(globalHandle, zone);
```

## Scalability Analysis



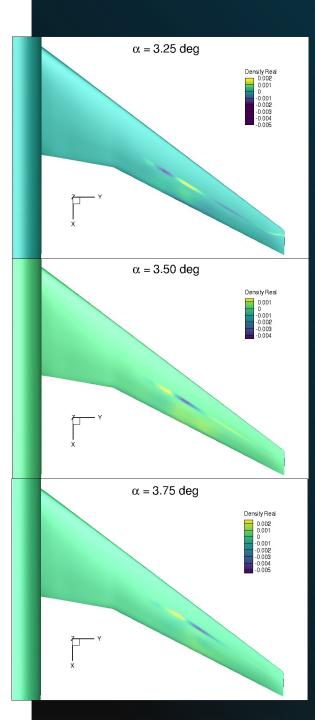
#### • Civil Airlines Model :

• CHAMPS' performance were similar to other softwares available industrially

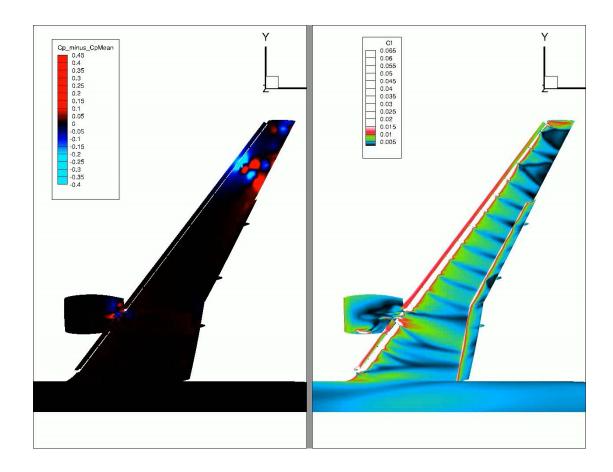
#### • Plain Box Model:

- Conducted on an **HPE HPC cluster** this test used a high number of cores (9216 cores in total) to explore CHAMPS's scalability.
- Tests with and without **reduction operations** revealed **super scalability** in the absence of reductions.

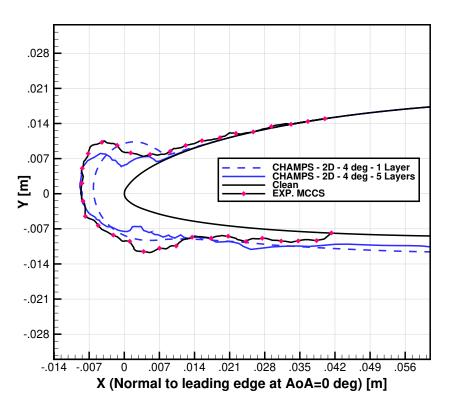
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- Predicting Ice shapes in 2D and 3D (IPW2)
- Multilayer Stochastic Ice accretion
- Lagrangian Model Scalability
- Aero-Elasticity



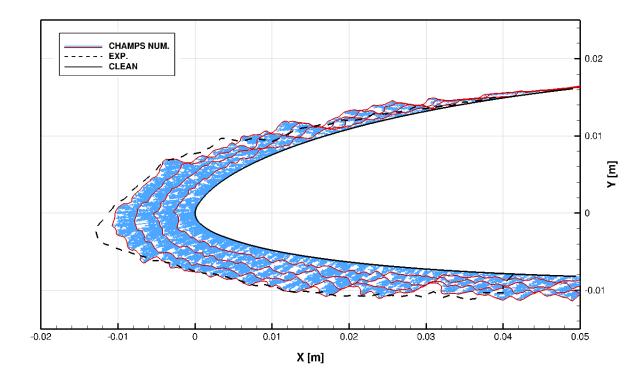
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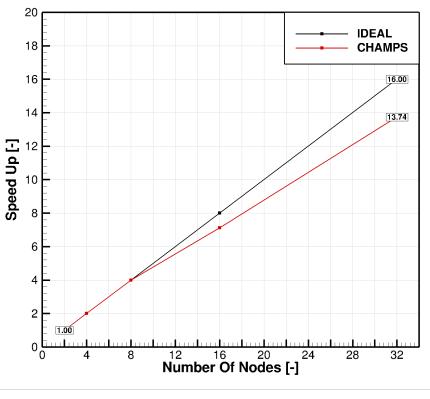
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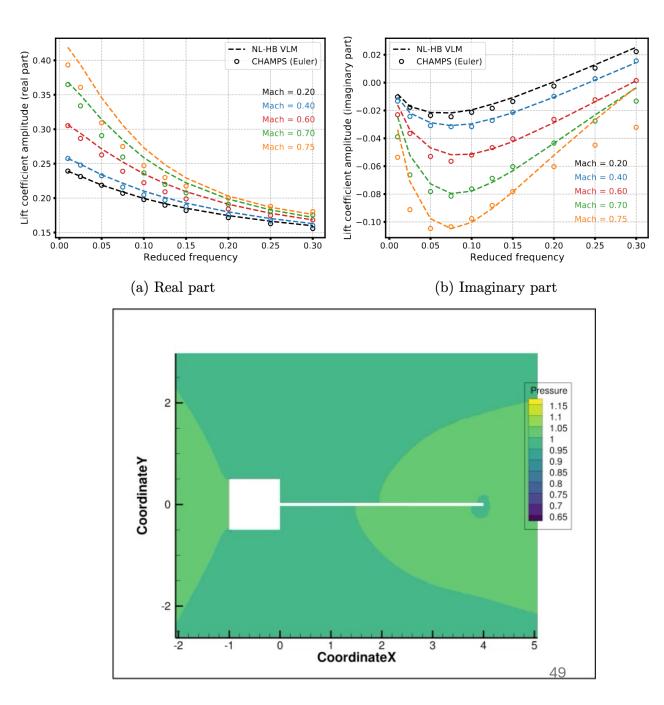


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1 Node = 40 Cores Total = 1280 Cores

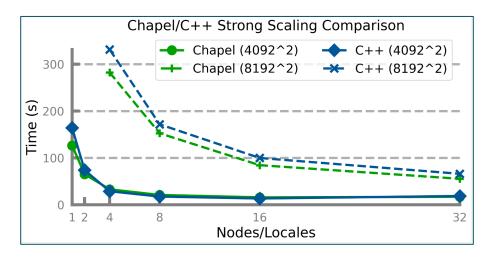
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## More on Chapel...

#### **Navier-Stokes in Chapel**

- Four introductory articles using Navier-Stokes as use-case
  - Based on an existing Python example
  - Chapel concepts are gradually introduced with side-by-side comparisons to Python
  - Basics of Chapel
  - Single-node parallelism
  - Introduction to distributed programming concepts
  - Ending with scalability and performance comparison with C++ / MPI



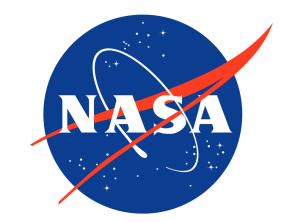


chapel-lang.org/blog/series/navier-stokes-in-chapel/



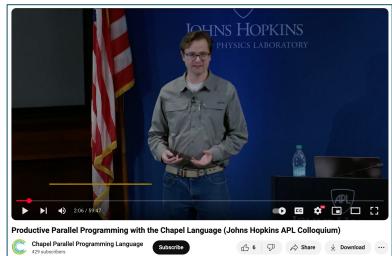
#### **A Pair of Previous Talks**

- Michael Ferguson (HPE) gave a talk at NASA Goddard
  - Productive Parallel Programming with the Chapel Language
  - A lot of performance comparisons to other languages
  - At-scale performance results using sorting
  - This talk may be available internally to you, as well



• A similar version from a Johns Hopkins University Applied Physics Lab Colloquium is available







#### 7 Questions for Chapel Users

Chapel Language Blog			Highly recommend Eric's interview on Chapel blog				
About Chapel W	Peakured Series T         7 Questions for Éu         Aircraft Aerodyna         Image: Chapel La         About Chapel Website F		Using Chapel in satellite image analysis for coral reef biodiversity analysis				
		7 Questions for Scott Bachman Coral Reefs with Chapel	: Analyzing			_	
		About Chapel Website Featured Serie	U	All Posts	Using Chapel in data analytics for atmospheri turbulence research in the Amazon		
	For the second secon			ws Data Analysis		Other success stories on graph processing and data analytics:	
					<u>chapel-lang.org/blog/series/7-questions-fo</u> stay tuned for more!	r-chapel-users/ 53	

#### Ways to Engage with the Chapel Community

#### **Live/Virtual Events**

- <u>ChapelCon</u> (formerly CHIUW), annually
- Office Hours, monthly
- <u>Live Demo Sessions</u>, monthly

#### <u>Community / User Forums</u>

- Discord
- **Discourse**
- Email Contact Alias
- GitHub Issues
- Gitter
- <u>Reddit</u>
- Stack Overflow

**D** Discord

III GITTER

( )

- C reddit
- stack overflow

chapel+qs@discoursemail.com

#### **Electronic Broadcasts**

- <u>Chapel Blog</u>, ~biweekly
- <u>Community Newsletter</u>, quarterly
- <u>Announcement Emails</u>, around big events

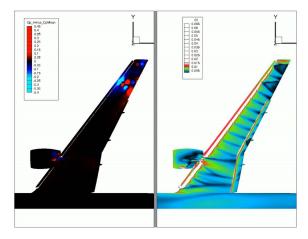
#### **Social Media**

- <u>Bluesky</u>
- Facebook
- Linked in • LinkedIn
- mastodon <u>Mastodon</u>
- <u>X / Twitter</u> X
- YouTube VouTube

#### **Closing Thoughts**

- Chapel is
  - productive,
  - parallel,
  - fast,
  - scalable,
  - open-source,
  - flight-proven 🙂
- Powered by Chapel, CHAMPS
  - is being developed very rapidly to increase its capabilities
  - can run on multiple nodes efficiently
  - produces high-fidelity results





Both teams are excited to hear comments, questions, and collaboration opportunities!

# Thank you