Parallel Applications Workshop, Alternatives to MPI+X

November 19^{th}, 2021

Held in conjunction with SC21: The International Conference for High Performance Computing, Networking, Storage, and Analysis

In cooperation with:

Our Panel

Barbara Chapman (HPE), OpenSHMEM

Alan Edelman (MIT), Julia

Eric Laurendeau (Polytechnique Montreal), Chapel

Modesto Orozco (IRB), Molecular Modelling and Bioinformatics

Nikhil Padmanabhan (Yale University), Physics and Astronomy

PAW ATM

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SC21 St. Louis, MO | science & beyond

TCHPC

Panel Goals

- Discussing real world applications that use other technologies for communication and computation
- Look at programming models and languages that are alternatives to MPI
- Understand strengths of these alternatives and applicability in the current HPC landscape
- Discuss obstacles in adopting these and find out how the community can help

OpenSHMEM

Barbara Chapman (HPE)

In cooperation with:

Julia

Alan Edelman (Massachusetts Institute of Technology)

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Aerospace Engineering

- National Objectives (Commercial & Defense)
- Flight testing extremely costly (Dollars and Humans)
- Simulation-Based Engineering have emerged from R&D (‘90s-2010’) to production
    - Disciplinary (manufacturing, aerodynamics, etc.)
- Technology push:
    - Multidisciplinary: link ‘fields’
    - fully coupled systems: link ‘software’
- Solution: democratizing HPC
    - Unified OS, languages, memory, architecture

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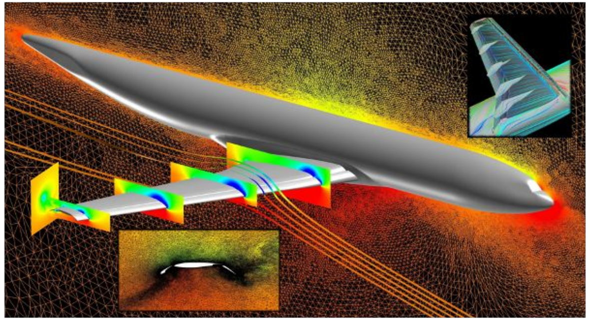
Aerodynamic Design Toolset

Bombardier

Flight tests~100 000$/hr

ETW

Wind-tunnel ~1000-10 000$/hr



NASA

Numerical Simulations (CFD)~100-1000$/hr

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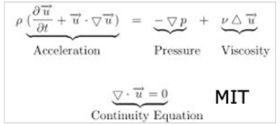
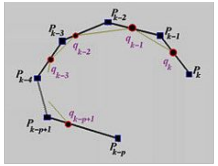
Workflow

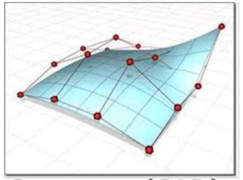
physics



mathematics

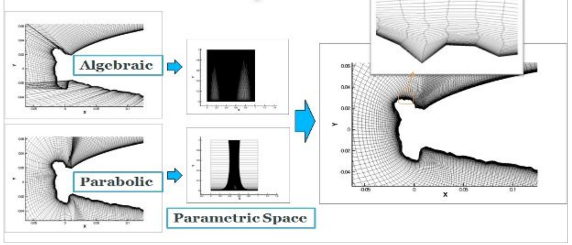


Parametrisation (NURBS)

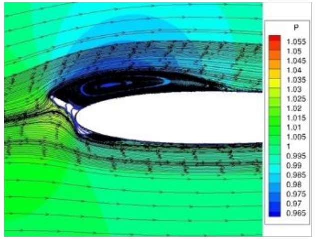


Geometry (CAD)

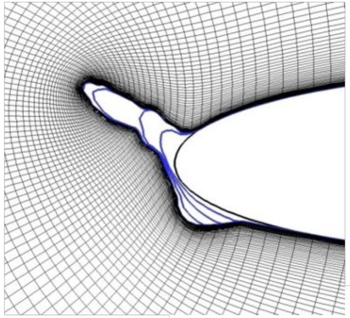
macro ➡ micro



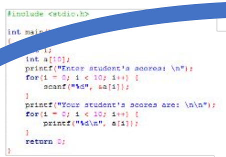
Mesh generation
0.01-10 billions unknowns



solution:
i) flow, ii) droplets



Time step



Proprietary source codes

Supercomputers

Enablers

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Education

- Technology used to be in academia
    - Research centers
        - Industry

- Handled by Professors, Research Associates, Post-Docs, highly specialized skill sets

- Now handled by MSc students
    - Push towards undergraduate training

- Example 1: Polytechnique Montréal adopted Python in all U.Grad courses (no more Matlab)
    - Python introduced at Bombardier through students! Technology push

- Example 2: Chapel used in 3D Navier-Stokes solver, will it see same success? (hopefully!)

Educational challenges

- Physics
- Applied Mathematics
- Numerical analysis
- Programming languages
- OPEN-MP (MSc)
- MPI (PhD, slow progress)
- Mixed CPU-GPU (failure in technology push)
- Time-to-debug (1 Million+ lines, 10 hrs runs)

How to you fit that:
-in U. Grad?
-in Ph.D. (with MSc dropping?)

So far, experience has shown Chapel is step change towards this goal.

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Molecular Modelling and Bioinformatics

Modesto Orozco (Institute for Research in Biomedicine (IRB) Barcelona)

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Chapel in Astronomy

Nikhil Padmanabhan (Yale University)

SC21
St. Louis, MO | science & beyond.

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Introduction

- Observational cosmologist
  - Use large galaxy surveys to constrain the underlying physics of the Universe - its initial conditions, and the nature of dark matter and dark energy
  - Inputs include both observational data as well as mock observations based on simulations.
  - Cosmologists are Bayesians - want to explore the posteriors, but likelihoods can often be expensive
- Not a traditional HPC use case, but analyses can quickly become computation-limited.
- Python has been the language of choice, normally supplemented with Cython/Numba/etc (and more recently Tensorflow/PyTorch etc).
  - Scaling : memory, multiple nodes
- Been using Chapel more and more in daily research, getting students more involved.
  - MPI bindings, initial prototype of c2chapel

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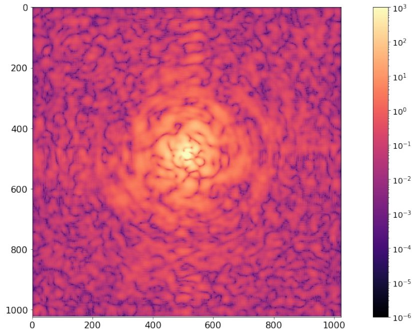
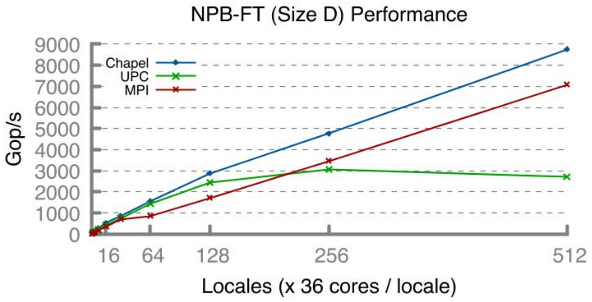
An example : chplUltra

- Explore the dynamics of ultralight dark matter.
- Solve a nonlinear Schrodinger equation
  - Pseudo-spectral solver
- History
  - Started as a port of a Python code
  - Initial shared memory version (directly interfaced to FFTW) easy, better performance compared to Python.
  - Multinode version required small changes to get working, reworked parallel FFT for performance.





NB: slab decompositions

w/ Luna Zagorac, Richard Easther
Zagorac et al, 2021

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Some thoughts

- Short-term research projects can be a fruitful ground for exploring alternatives.
  - Do not have the inertia of large legacy applications
- Big single multicore nodes now quite normal, nice to be able to scale out to multiple nodes/accelerators with small changes to code
- Lots of time/code spent doing “other” steps, important for the language to be expressive enough to handle these.
- Impedance matching with OpenMP+MPI.
- Interfacing with Python and friends.
- Community matters!