Petascale Adaptive Computational Fluid Dyanamics

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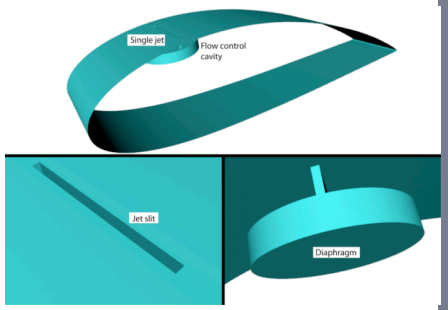
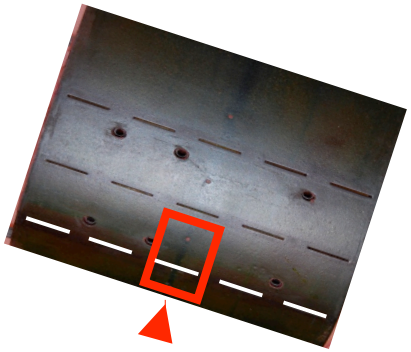
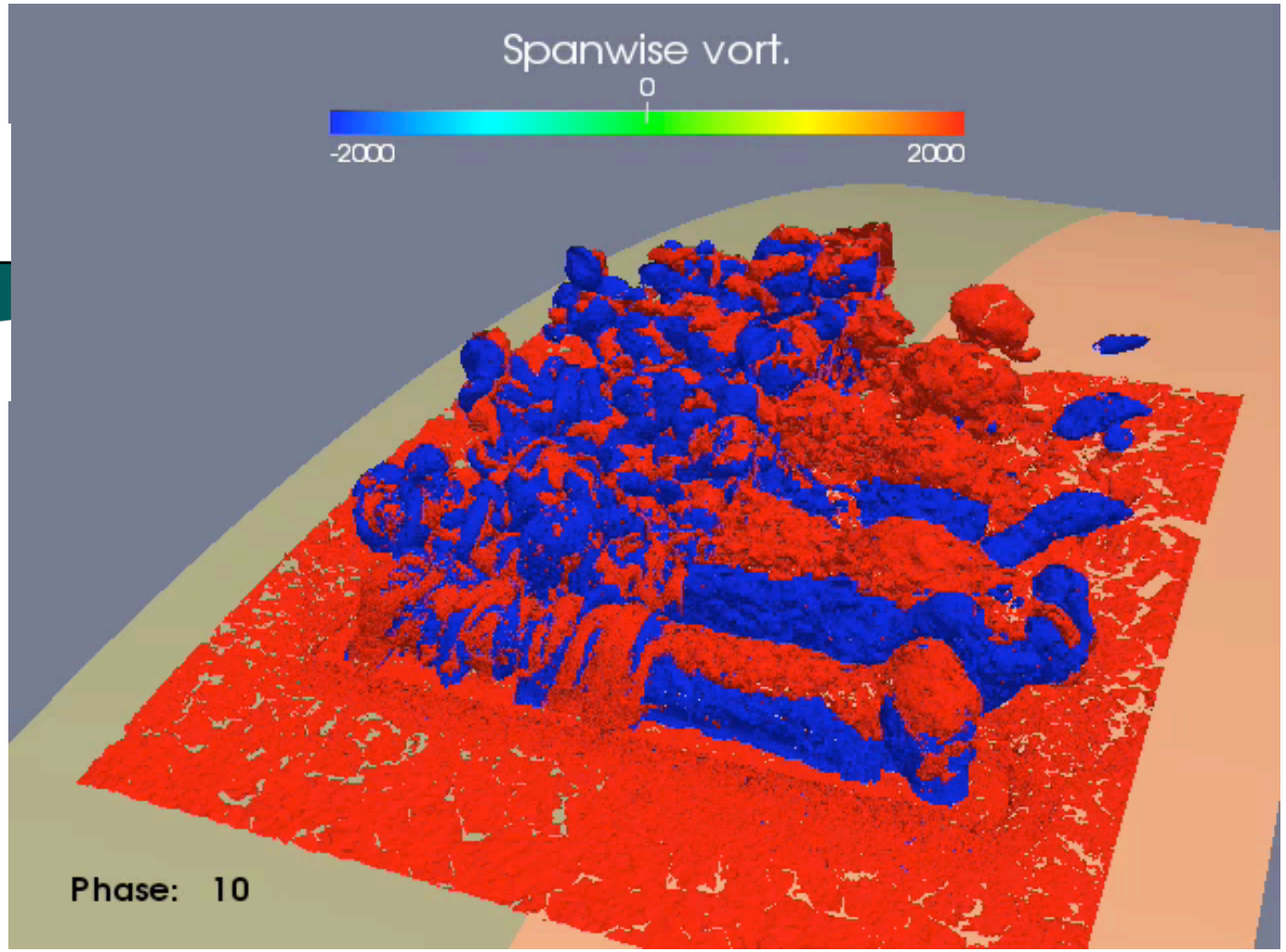
Sponsors: DOE: SciDAC-ITAPS, NERI; NSF: PetaApps, ITR, CTS; AFOSR, IBM, Northrup Grumman, Boeing, Lockheed Martin, Motorola
Computer Resources: INCITE (ANL, ORNL), TeraGrid (TACC,NICS), JSC, RPI-CCNI

Problems of Interest

Aerodynamic Flow Control

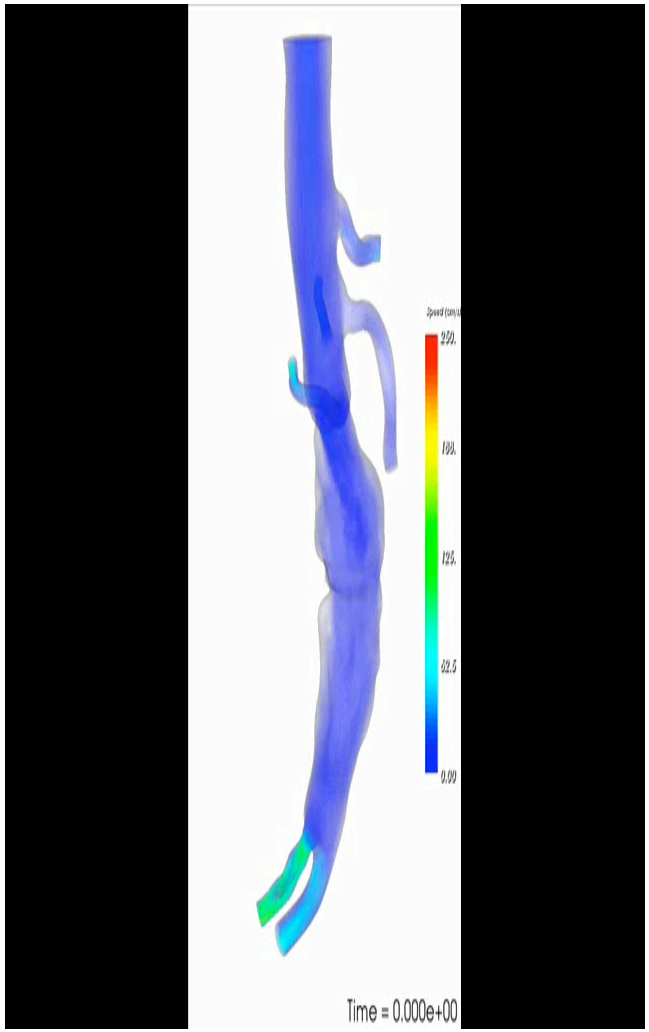






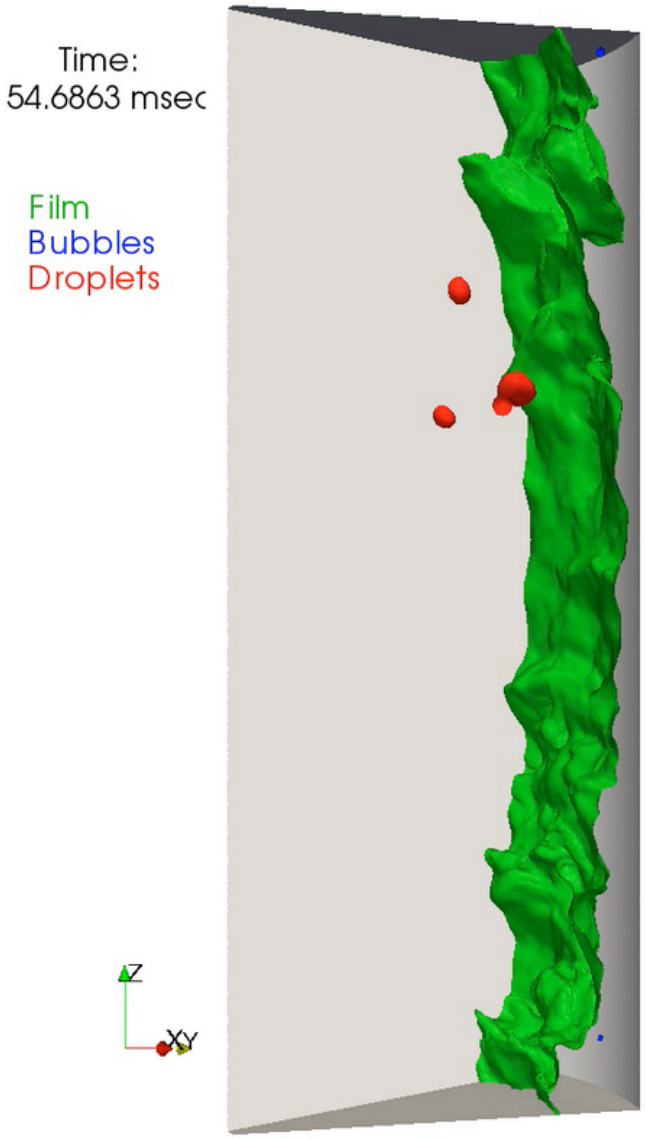
Problems of Interest

Cardiovascular flow: Abdominal Aorta Aneurysm



Problems of Interest

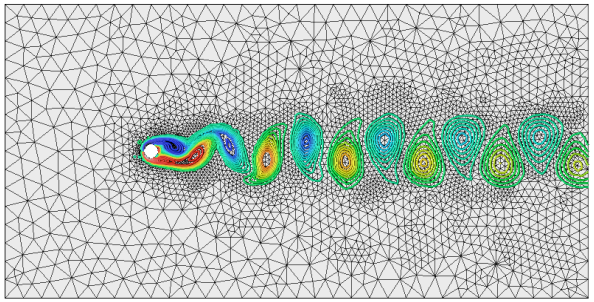
Two-phase
Annular Flow
(level set method)



PHASTA Flow Solver

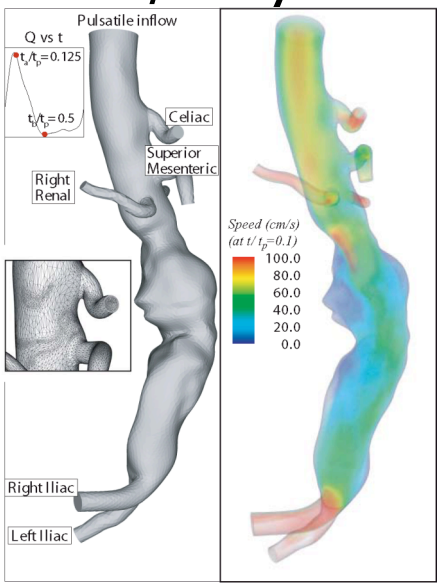
- Parallel Hierarchic Adaptive Stabilized Transient Analysis

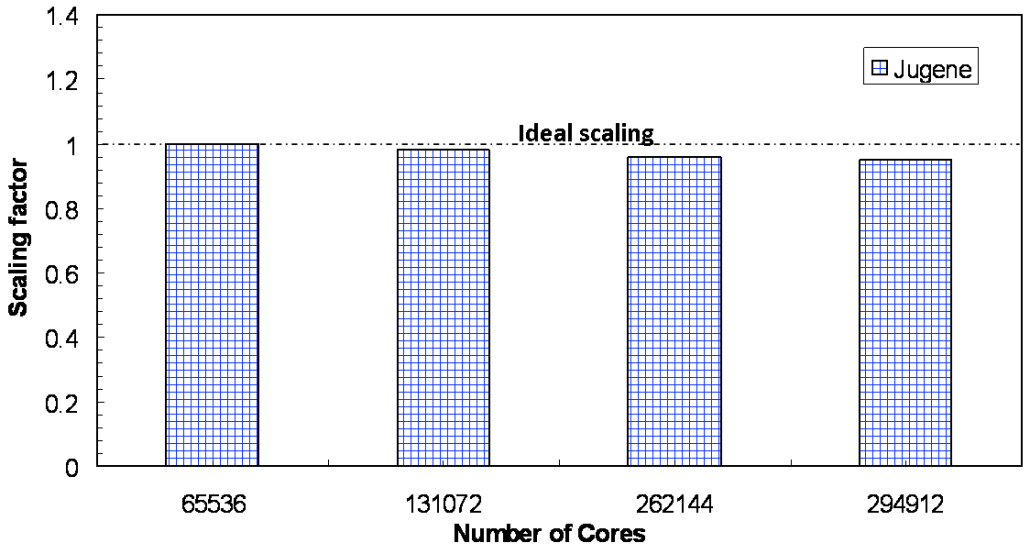
- Stability with Accuracy
  - Time accurate stabilized finite element method
  - Hierarchic spatial basis (currently p<4) $O(h^{p+1})$
  - Time integration: implicit (2^{nd} order generalized alpha method).
- Adaptivity
  - Grid matches physical scale
  - Anisotropic and transient
- Parallel
  - Excellent scaling to 288k processors (95%)



Strong Scaling – 5B Mesh up to 288k Cores

- AAA 5B elements: full-system scale on Jugene (IBM BG/P system)





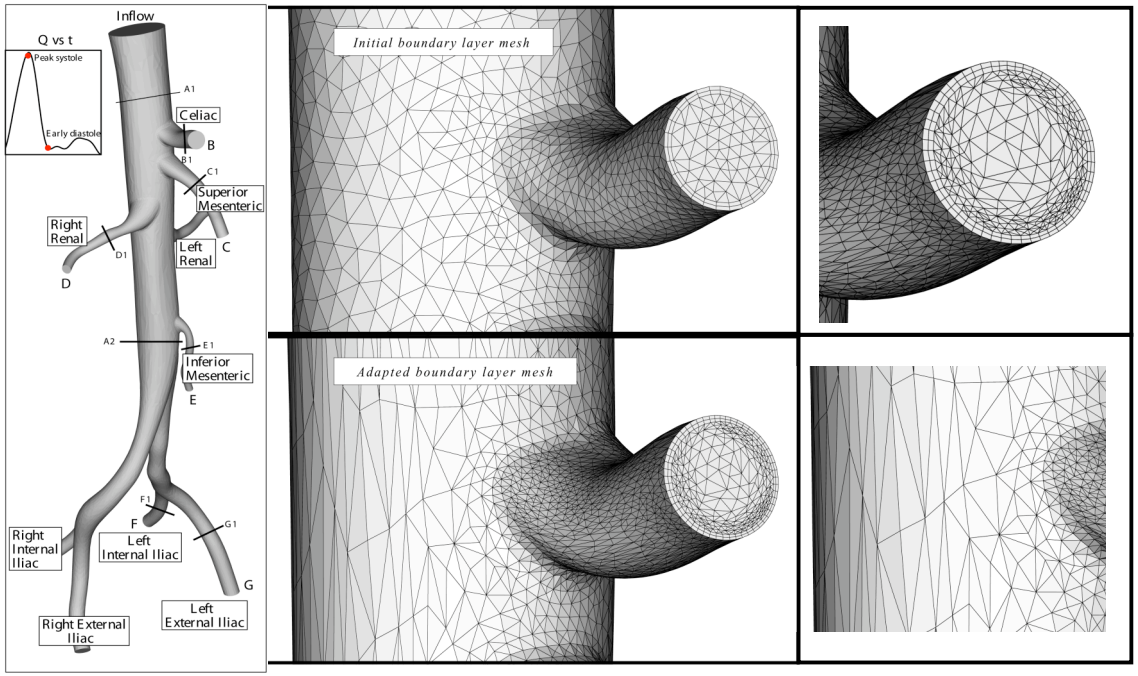
5B elements mesh (Jugene:IBM BG/P)		Eqn. form.		Eqn. soln.		Total	
num. of core	avg. elem./core	time	s-factor	time	s-factor	time	s-factor
65,536 (base)	76,480	119.64	1	162.59	1	288.23	1
131,072	38,240	59.69	1.00	84.09	0.97	143.78	0.98
262,144	19,120	30.02	1.00	43.24	0.94	73.26	0.96
294,912	16,995	26.71	1.00	39.15	0.92	65.86	0.95

without IPMod strong scaling factor is **0.88** (time is 70.5 secs),
for production runs savings can be in **43 cpu-years**

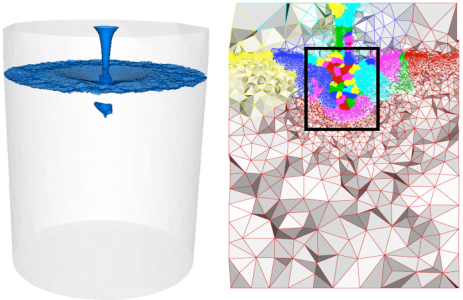
Current Approach – Unstructured Meshes

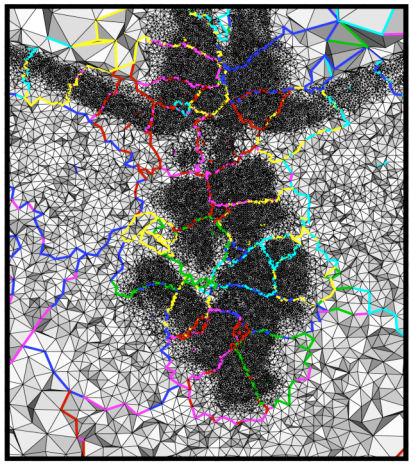
- Flow solver is designed to use general unstructured, anisotropic meshes; current meshes are constructed using parallel adaptive meshing capable to handle arbitrary complex geometry:

Healthy human aorta
(with adapted boundary layer mesh)

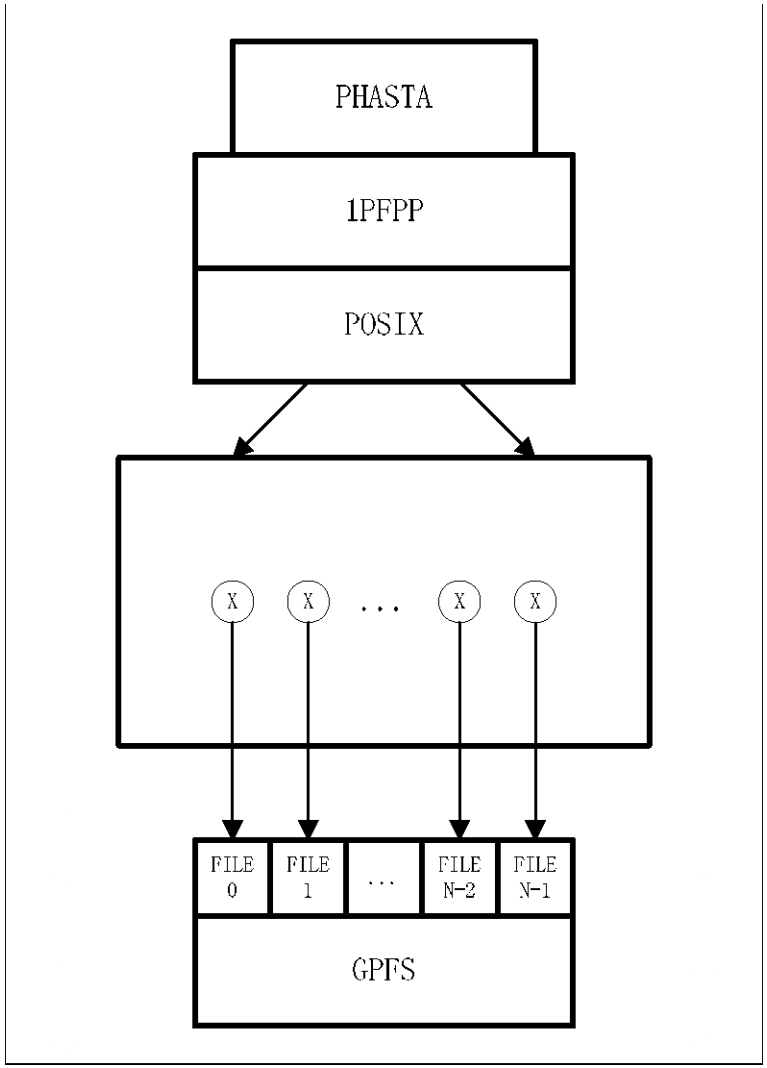


Plunging liquid jet
(colors indicate parts of a partitioned mesh)



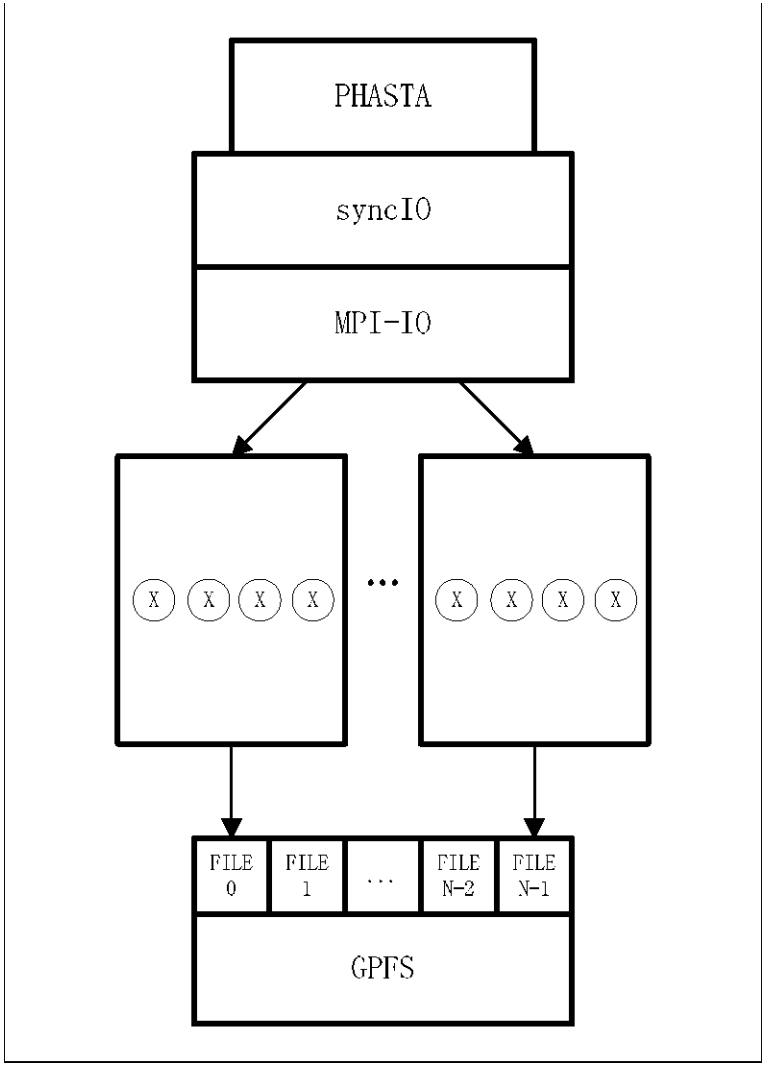


OLD I/O: 1 POSIX File Per Processor



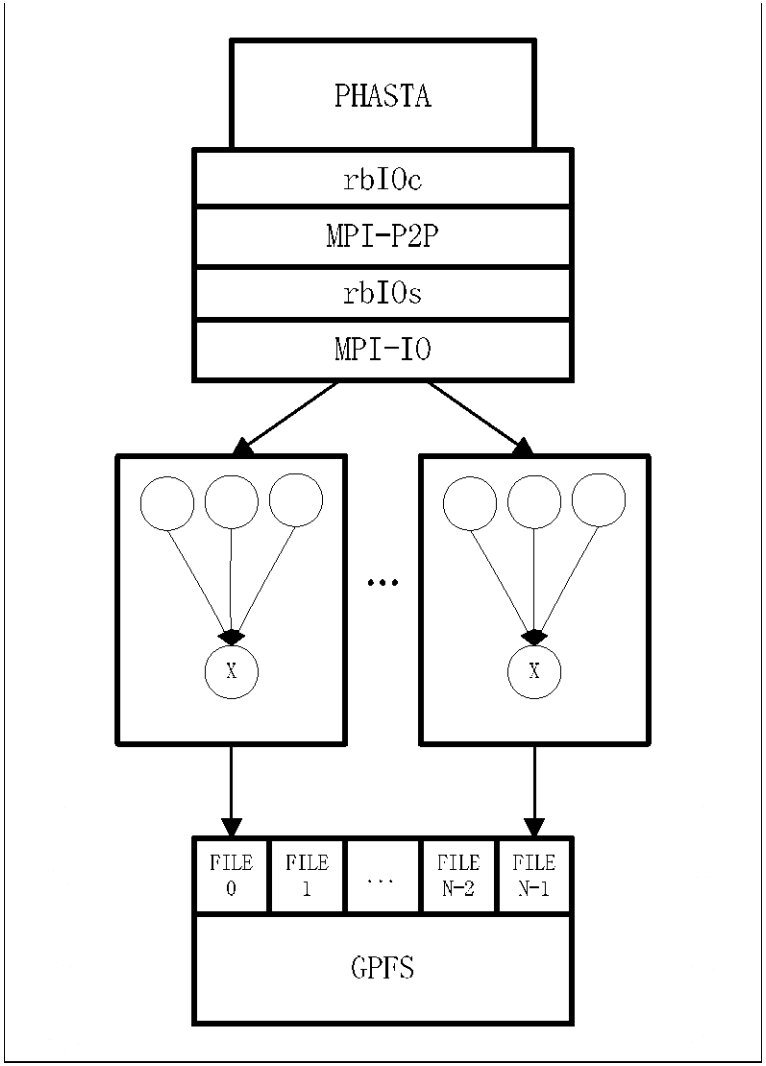
- Pros:
  - parallelism, high performance at small core counts
- Cons:
  - lots of small files to manage
  - LOTS OF METADATA – stress parallel filesystem
  - difficult to read back data from different number of processes
  - @ 300K cores yields 600K files
    - @ JSC ➔ kernel panic!!
  - PHASTA currently uses this approach…
- < 1 GB/sec on BG/L

I/O: MPI_File alternatives and syncIO



- Flexible design allows variable number files and procs/writers per file
- Within a file, can be configured to write on "block size boundaries" which are typically 1 to 4MB.
- Implemented using collective I/O routines : e.g., MPI_File_write/read_at_all_begin
- BG/P: 11.6 GB/sec read,
  25 GB/sec write

I/O: MPI_File alternatives and rbIO



- Rb ➔ "reduced blocking"
- Targets "checkpointing"
- Divides application into workers and writers with 1 writer MPI task per group of workers.
- Workers send I/O to writers over MPI_Isend and are free to continue –
  - e.g., hides the latency of blocking parallel I/O
- Writers then perform blocking MPI_File_write_at operation using MPI_COMM_SELF communicator
- BG/P: ~18 GB/sec actual write,

~167 TB/sec perceived write @ 128K cores

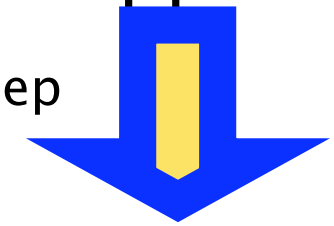
- So long as the workers do not request another write before writers complete, there is a big efficiency gain.

  Writer pool can be sized to achieve this.
- Can we message directly I/O nodes?

In situ vizualisation

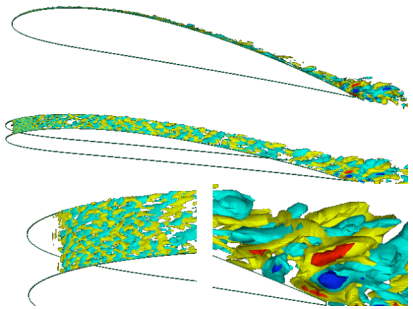
- Kernel of ParaView has been linked into PHASTA on N processors.
- Filter chain defined on interactive client and saved
- Filter chain executed at user prescribed frequency
    - Current solution, coordinates and connectivity passed from PHASTA to ParaView
    - ParaView executes filter chain on N processors, collects filter output geometry and transfers (by sockets or files) to PVServer running on n cores of a viz cluster
    - Geometry rendered on viz nodes and displayed on a local ParaView Client
- Currently scales reasonably well on N=8k cores on BGL at CCNI
- Work underway to extend to Intrepid-Eureka with N=160k
- Should work for VisIt too.

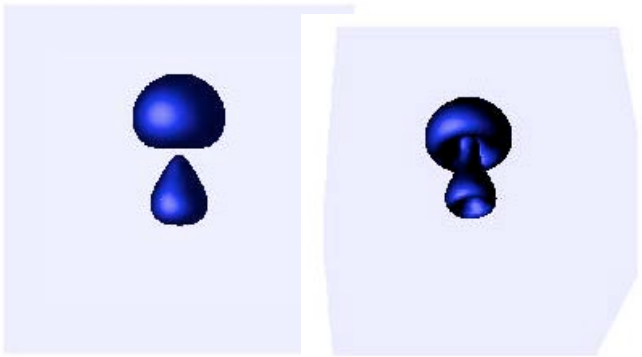
Summary

- Complex geometry/physics=> Real world Apps
- Implicit solvers: Complexity  but n_{step} 
- Excellent scaling results
- Big Science AND FAST SCIENCE
- Anisotropic Adaptivity brings real geometry problems into reach of solution in a USEFUL time frame
- Multiphase simulation capable of modeling turbulent flow with mixture of steam and water
- Complex geometry of very small flow control devices being simulated and validated.
- Patient-specific cardiovascular flows can be solved in clinically relevant time frame.

PHASTA Models

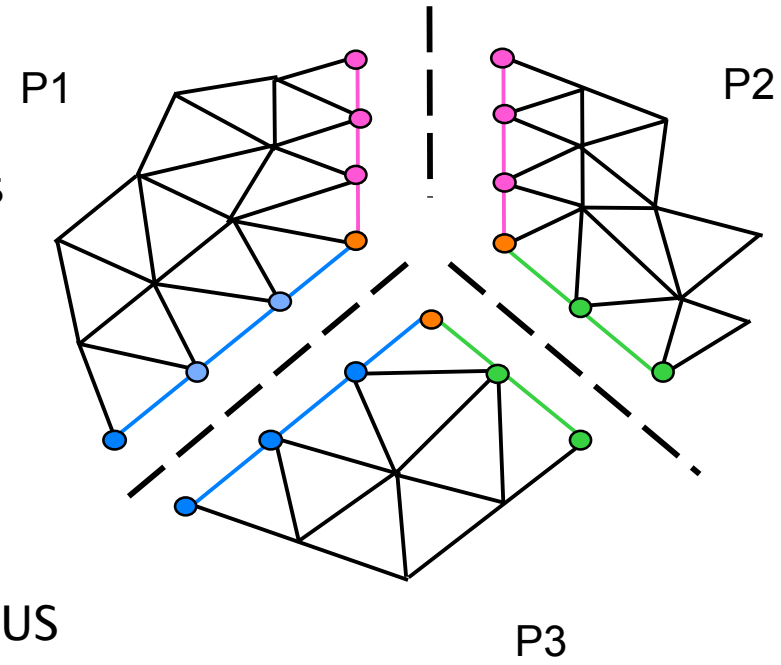
- Compressible or Incompressible flow solver
- Turbulence
  - Direct Numerical Simulation (DNS)
  - Large-Eddy Simulation (LES)
  - Reynolds-Averaged Navier-Stokes (RANSS)
  - Detached Eddy Simulation (DES) and other hybrid models





PHASTA Flow Solver Parallel Paradigm

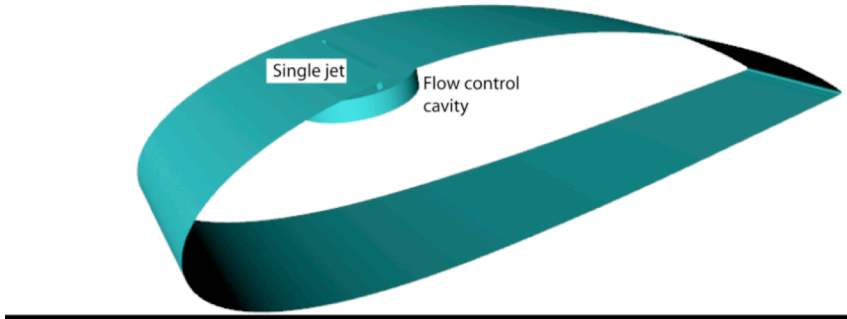
- Implemented in Fortran/C++ & MPI
- Input partitioned on a per-processor basis
- Unstructured mesh "parts" mapped to cores
- Two types of work:
  - **Equation formation (Ax=b)**
    - Matrix assembled on processor ONLY
    - O(40) peer-to-peer non-blocking comms to update share dofs in **b**
    - Scales well on many machines
    - Cost ÷ number of elements
  - **Implicit, iterative equation solution**
    - For each Krylov vector:
      - q=Ap (matrix-vector products)
      - Same peer-to-peer comm as **b** for **q** PLUS
      - Orthogonalize against prior vectors
      - **REQUIRES NORMS=>MPI_Allreduce**
      - Cost ÷ number of nodes

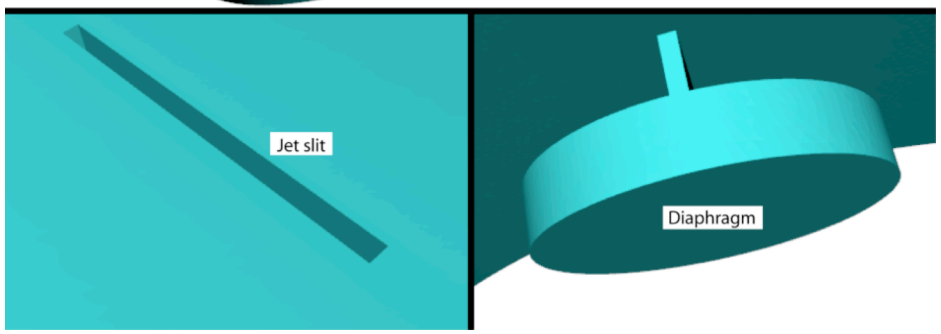


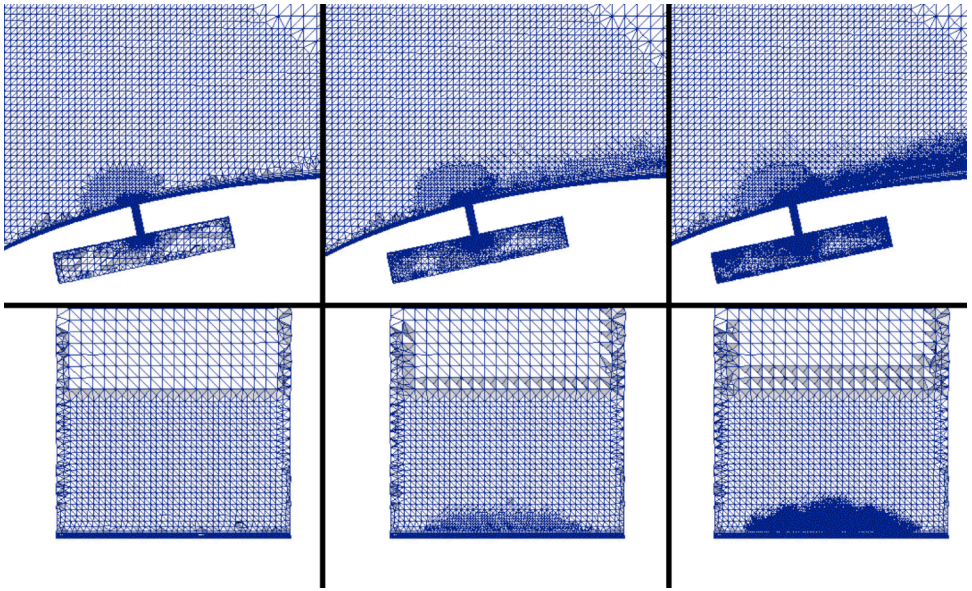
- **I/O**: Initial read of mesh data + Checkpoint after "N" interations

Finite-span synthetic jets

CAD geometry used in CFD matches experiment







Initial and 2 cycles of adapted mesh
Spanwise slice (top)
Streamwise slice 20 slit widths down stream (bottom)