Construction of Parallel Adaptive Simulation Loops

FASTMath Team Members: Brian Granzow[1], Glen Hansen[2], Dan Ibanez[1], Cameron Smith[1], E. Seegyoung Seol[1], Max Bloomfield[1], Andrew Bradley[2], Dan Zaide[1], Onkar Sahni[1], Mark S. Shephard[1] [1]SCOREC, Rensselaer Polytechnic Institute [2]Sandia National Laboratories

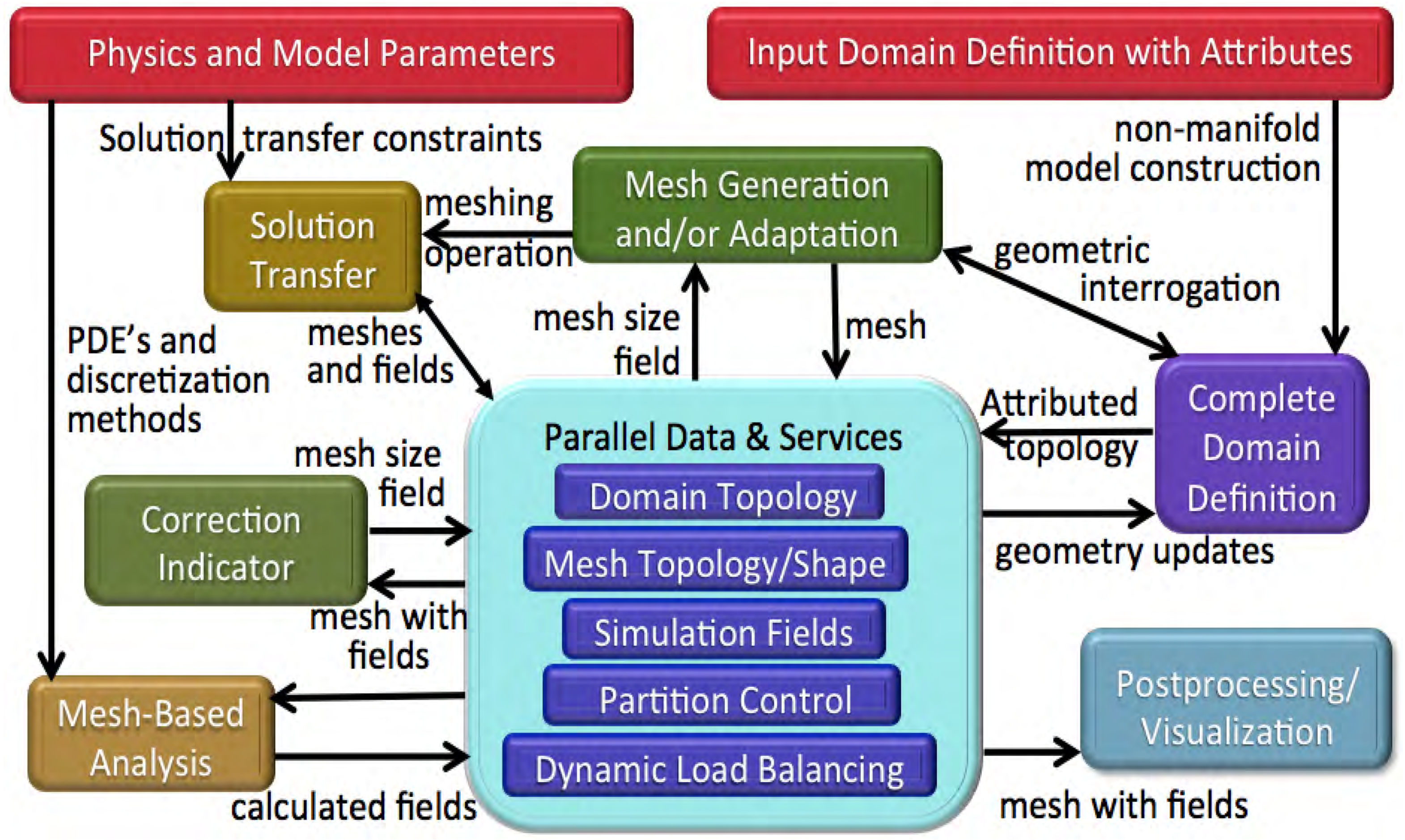
The automation of large-scale reliable simulations requires the integration of a number of components within an adaptive mesh loop that can maintain scalability. Components to support these operations on massively parallel computers have been developed and have been integrated in-memory with multiple unstructured finite element and finite volume codes.

Parallel Adaptive Loops

Goal is automated, reliable, scalable, massively parallel simulations

- Automation – automatic mesh generation, in-memory integration of components eliminates manual user intervention
- Reliability – solution accuracy ensured via error indicators and mesh adaptation
- Component based – flexibility through different components
- Efficiency – all components run on the same machine, in-memory integration eliminates file i/o, predictive load balancing

Parallel Adaptive Simulation Workflows



Adaptive Loop Applications

Adaptive loops to date have been used to solve

- Modeling of nuclear accidents and various flow problems with University of Colorado Boulder's PHASTA code
- Solid mechanics applications with Sandia's Albany code
- Fusion MHD with PPPL's M3D-C1 code
- Accelerator modeling problems with SLAC's ACE3P code
- Aerodynamics problems with NASA's Fun3D code
- Waterway flow problems with ERDC's Proteus code
- High-order fluids simulations with Nektar++

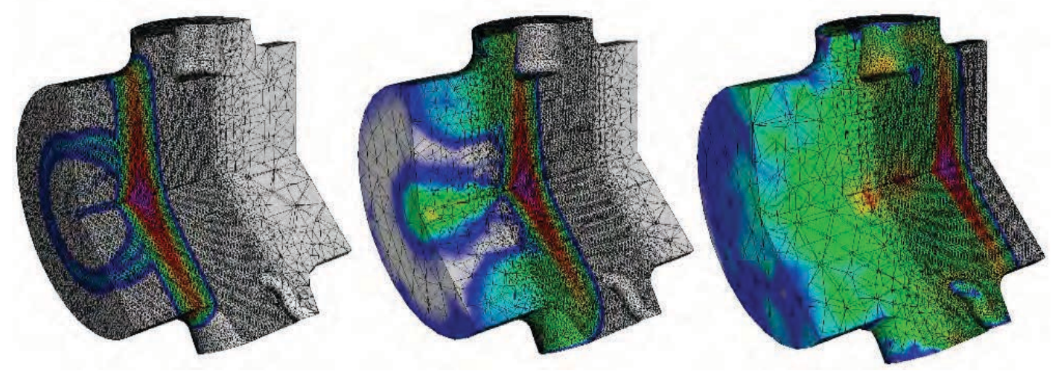
Adaptive Loop Components

Purpose	Software Components
CAD Geometry	Parasolid, ACIS, Simmetrix
Mesh Generation	Simmetrix, Gmsh
Mesh Database	PUMI (SCOREC) – parallel unstructured mesh infrastructure
Geometric Queries	GMI (SCOREC) – geometry interface
Analysis Codes	PHASTA (Univ. Colorado Boulder), Albany (Sandia), M3D-C1 (PPPL), ACE3P (SLAC), Fun3D (NASA), Proteus (ERDC), Nektar++ (Imperial)
Mesh Adaptation	MeshAdapt (SCOREC), Simmetrix
Load Balancing	ParMA (SCOREC) – diffusive load balancing, Zoltan2 (Sandia)
Field Data	APF (SCOREC) – field storage and transfer
Error Estimation/ Indication	SPR (SCOREC) – projection based, DWR (SCOREC) – goal oriented

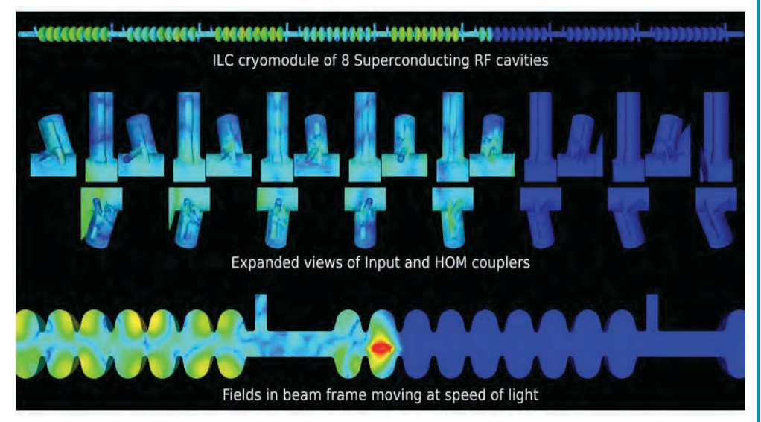
Library Based In-Memory Integration

Component implementation drives component coupling approach

Serialized data streams using existing file reading and writing protocol



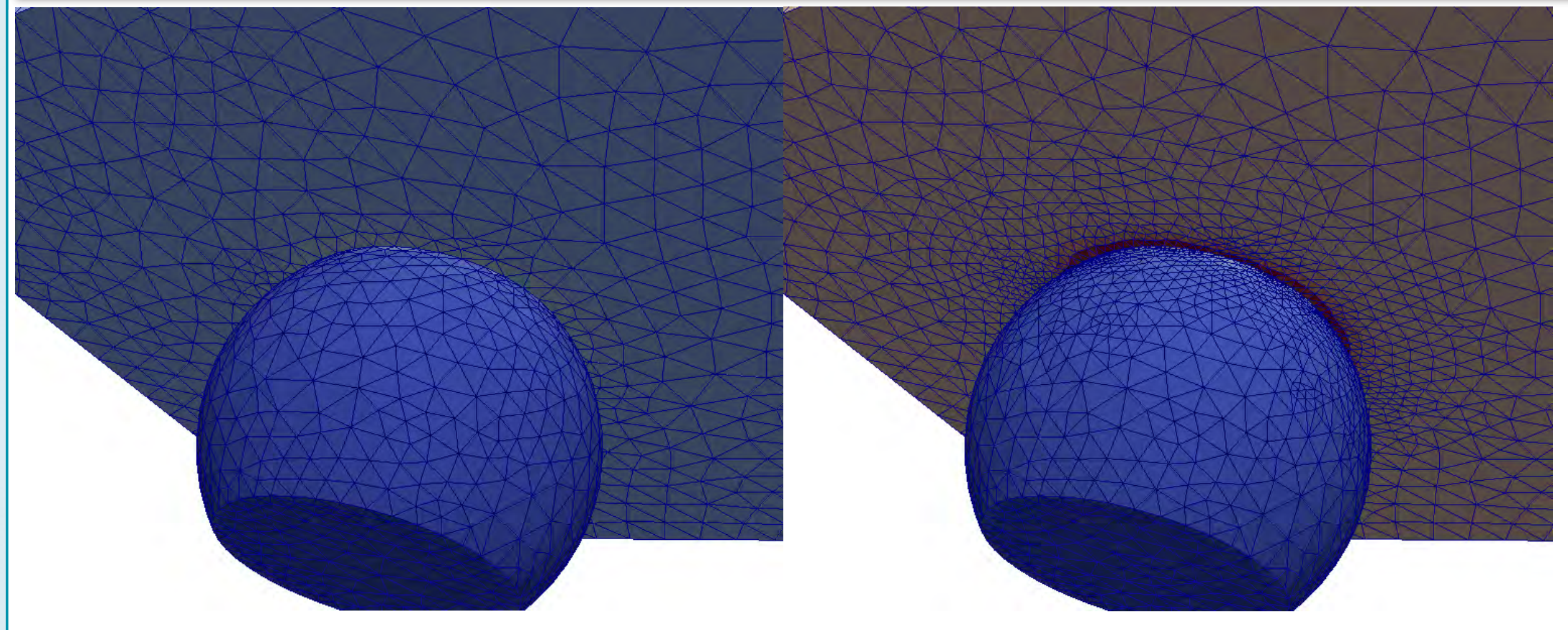
- Minimal code changes
- Ideal for components already coupled via files
- Logical choice for uncoupled components with I/O support and without data APIs – interacting components implement I/O protocol


SLC cryomodule of 8 Superconducting RF cavities
Expanded views of input and HOM couplers
Fields in beam frame moving at speed of light

API based transfer procedures

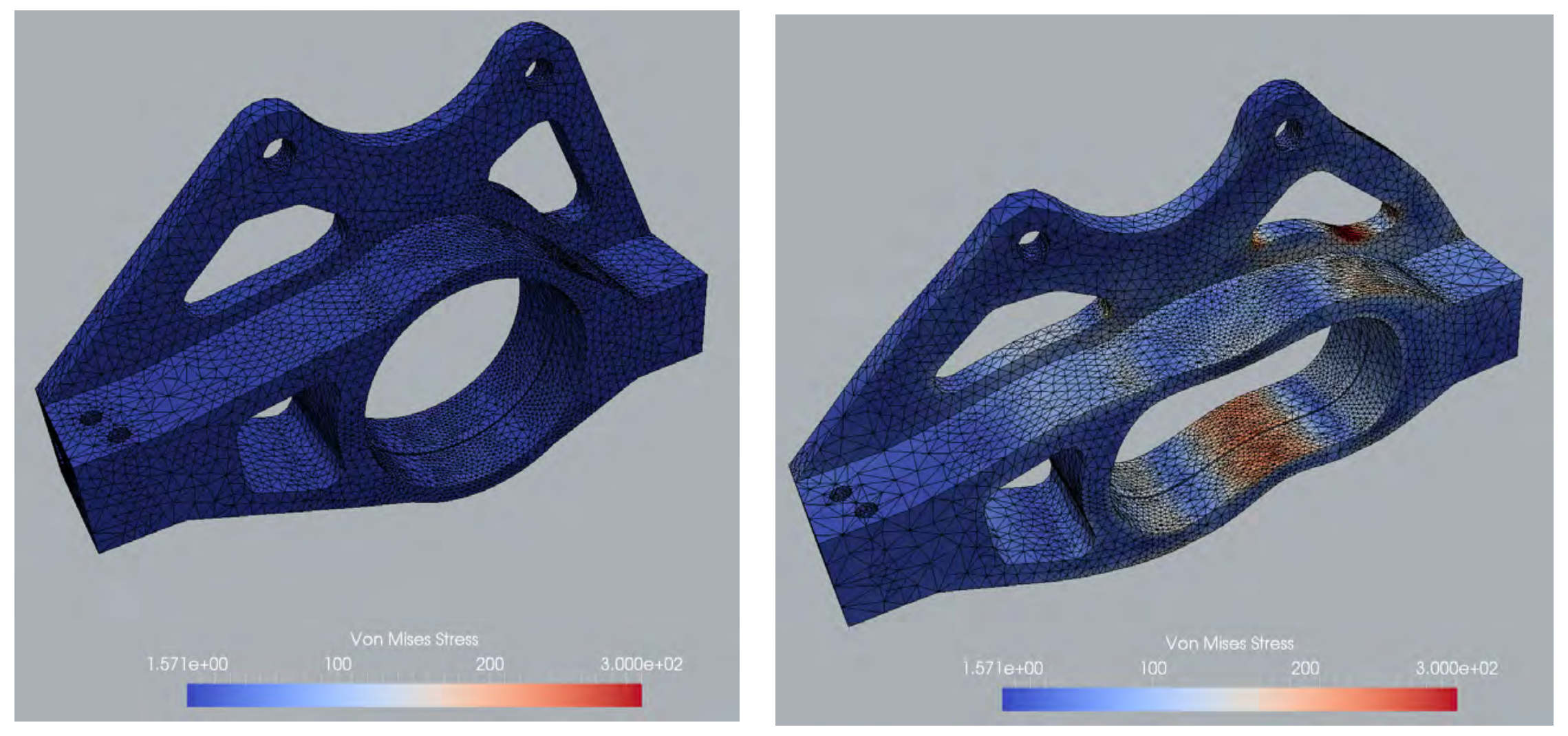
- Flexibility to extend functionality via passing additional information or control parameters
- Supports common data representation – reduced memory usage
- Ideal for components with APIs that support querying and modifying data structures
- Logical choice for components already coupled via files that want access to data from multiple components – replace I/O procedures with API calls populate data structures

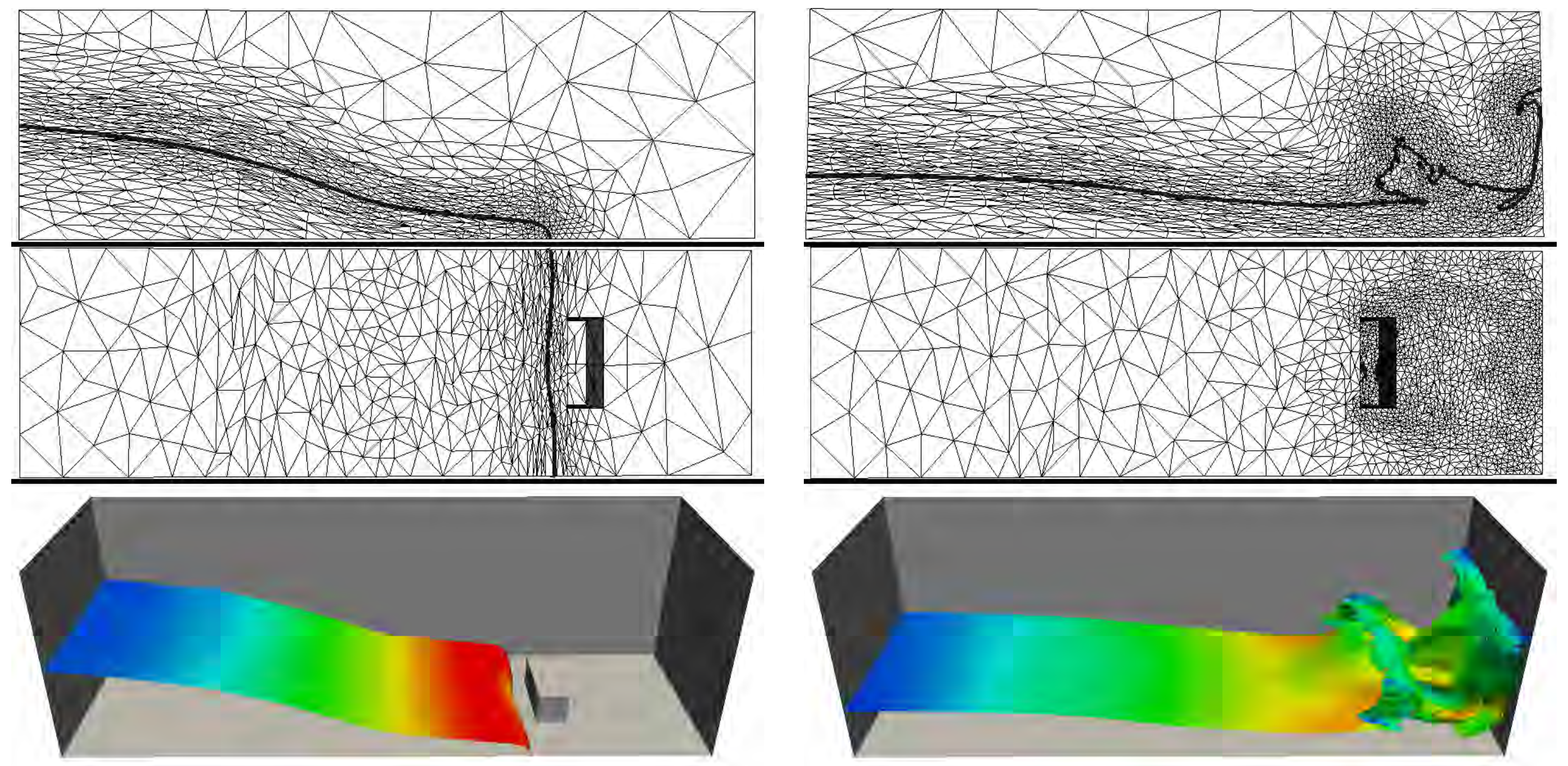
Adaptive Loop Applications



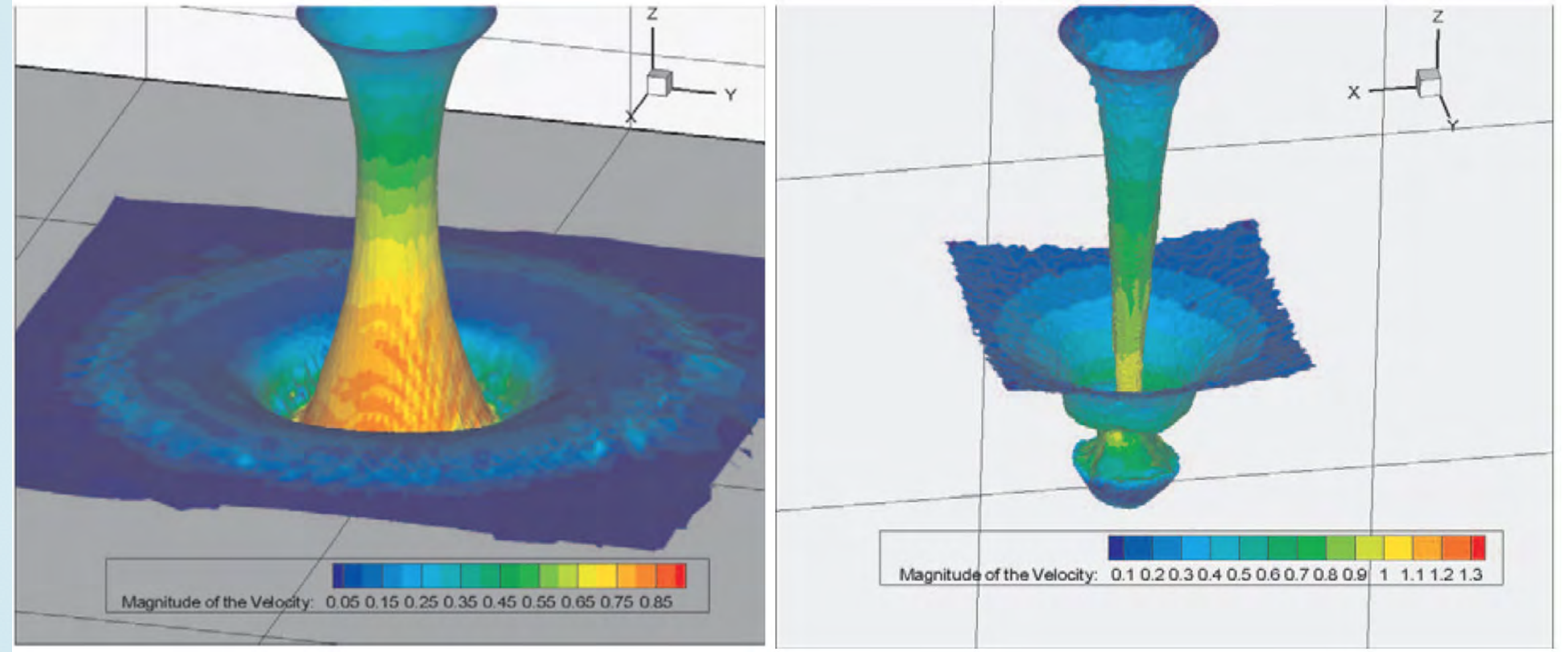
In-memory integration of the adaptive loop components with Albany (Sandia) to model creep and plasticity in a stressed solder ball to predict mechanical failure in flip chip packaging

An automotive upright subject to large deformations using integration of the adaptive loop components with Albany (Sandia). Initial mesh (right) and adapted mesh after 20 load steps (left)





Simulation of a dam break with obstacle using in-memory anisotropic adaptive loop with Proteus (ERDC). (Top) Mesh cross-section from a side view. (Middle) Mesh cross-section from a top down view. (Bottom) Fluid interface with velocities



Simulation of a plunging liquid jet using in-memory integration of the adaptive loop with PHASTA (Colorado). (Left) Liquid interface at 0.075s. (Right) Liquid interface at 1.3075s

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