Section 6
Service Components

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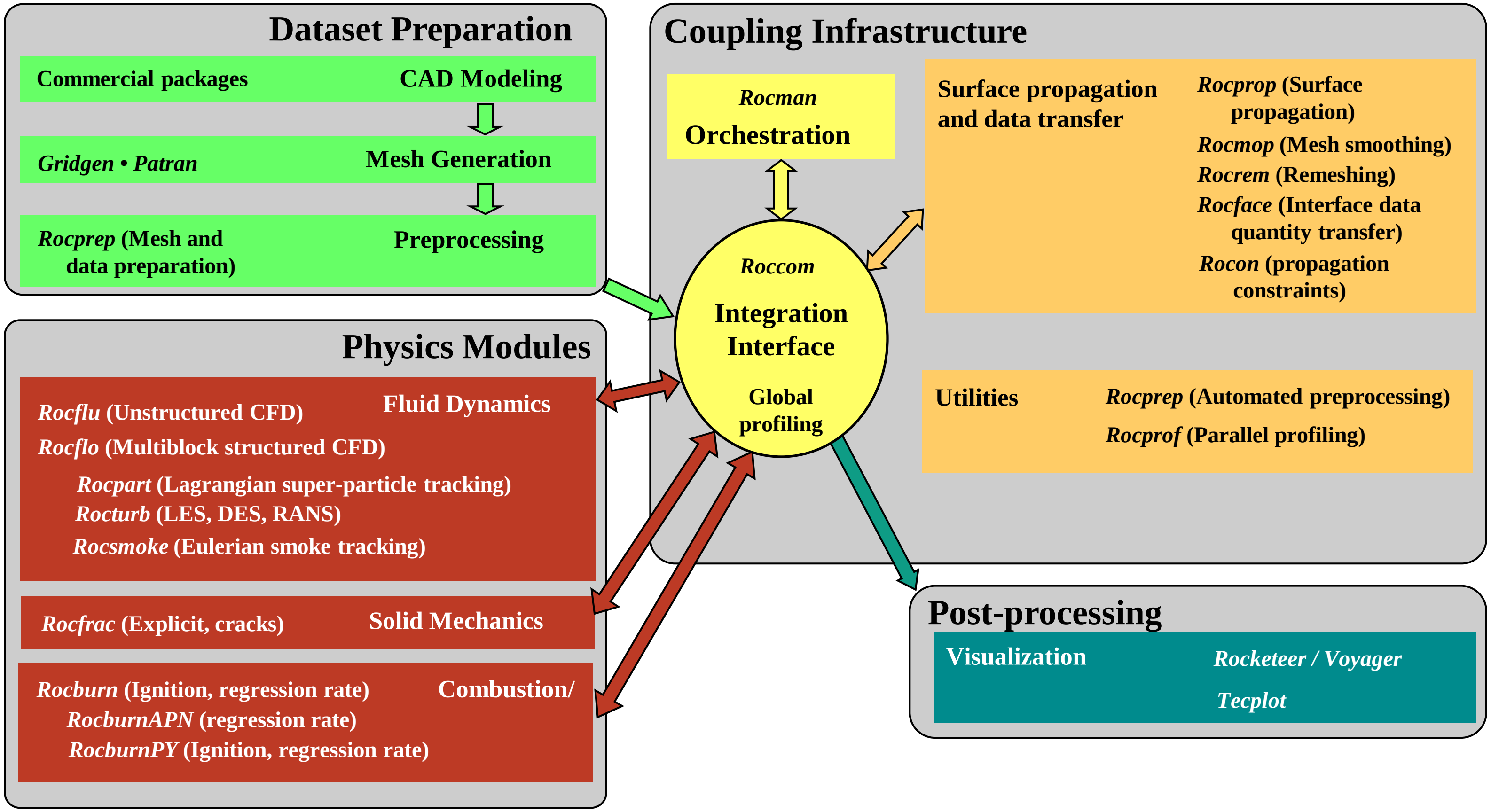
Rocstar Simulation Suite Architecture



Dataset Preparation

Commercial packages — CAD Modeling

Gridgen • *Patran* — Mesh Generation

Rocprep (Mesh and data preparation) — Preprocessing

Coupling Infrastructure

Rocman
Orchestration

Roccom
Integration Interface
Global profiling

Surface propagation and data transfer

- *Rocprop* (Surface propagation)
- *Rocmop* (Mesh smoothing)
- *Rocrem* (Remeshing)
- *Rocface* (Interface data quantity transfer)
- *Rocon* (propagation constraints)

Utilities

- *Rocprep* (Automated preprocessing)
- *Rocprof* (Parallel profiling)

Physics Modules

Fluid Dynamics

- *Rocflu* (Unstructured CFD)
- *Rocflo* (Multiblock structured CFD)
- *Rocpart* (Lagrangian super-particle tracking)
- *Rocturb* (LES, DES, RANS)
- *Rocsmoke* (Eulerian smoke tracking)

Solid Mechanics

- *Rocfrac* (Explicit, cracks)

Combustion/

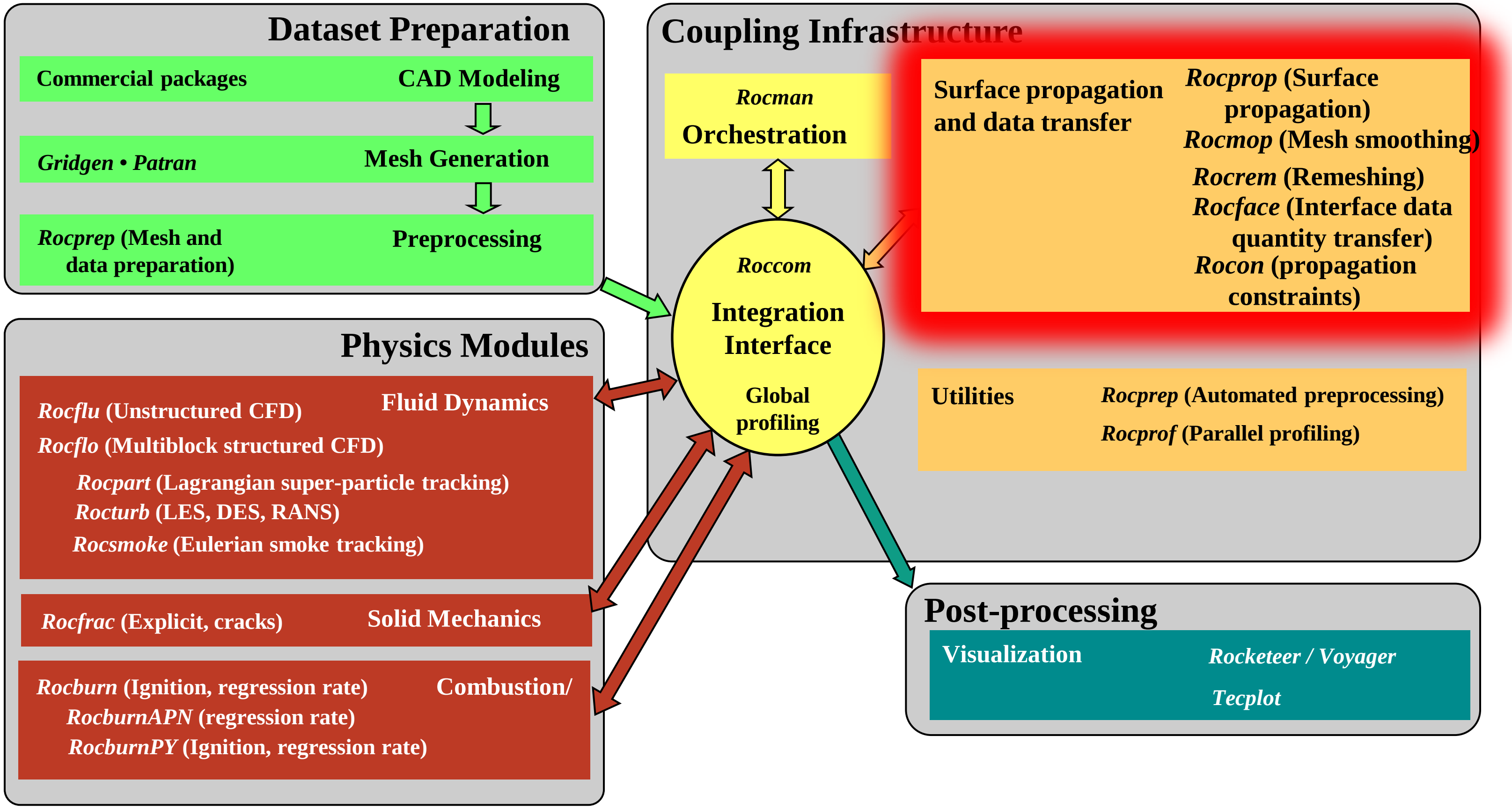
- *Rocburn* (Ignition, regression rate)
- *RocburnAPN* (regression rate)
- *RocburnPY* (Ignition, regression rate)

Post-processing

Visualization

- *Rocketeer / Voyager*
- *Tecplot*

Rocstar Simulation Suite Architecture



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Surface propagation and data transfer: *Rocprop* (Surface propagation), *Rocmop* (Mesh smoothing), *Rocrem* (Remeshing), *Rocface* (Interface data quantity transfer), *Rocon* (propagation constraints)

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Multiphysics Simulation Service Utilities

- Middleware services
  - IO: screen, disk
  - Mesh-level communication: point to point, collectives
  - Intermodule mesh/processor mapping
  - Control callbacks
- Numerical services
  - Data transfer: Surface-surface, volume-volume (abutting, overlapping)
  - Algebraic manipulation: data massaging, unit conversions, etc
- Geometric services
  - Mesh optimization: Mesquite-based
  - Surface propagation: Entropy conserving Lagrangian
  - Data structures: facilitate general service constructions

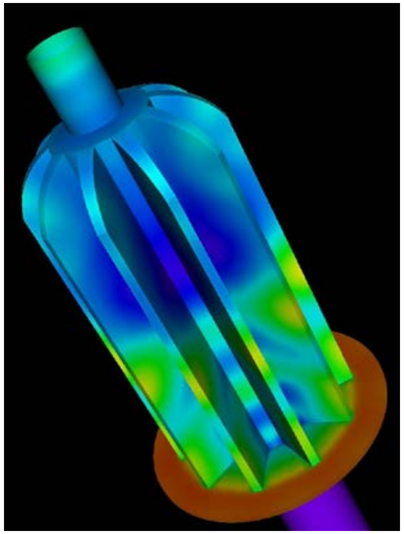
I/O and Control Services

- I/O Services
  - Disk I/O
    - Periodic snapshots for visualization and restart
    - Simple high-level interface
    - Collective output with active buffering
    - Parallel non-blocking
    - Multiple file formats (HDF/CGNS)
  - Screen I/O
    - Stdout/stderr (logged or to screen)
    - Parallel debugging logs
    - Automatic module tagging

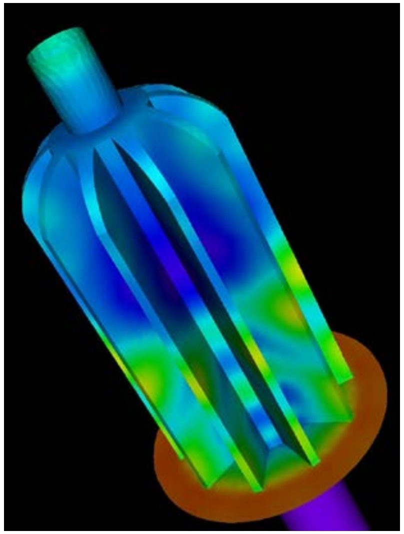
- Control flow services
  - Allows clean system interrupts
  - Prevents premature exits from batch system
  - Implemented as callbacks
    - Stop simulation
    - Restart simulation
    - Force checkpoint
    - Request domain remeshing

Communication between Physics Codes

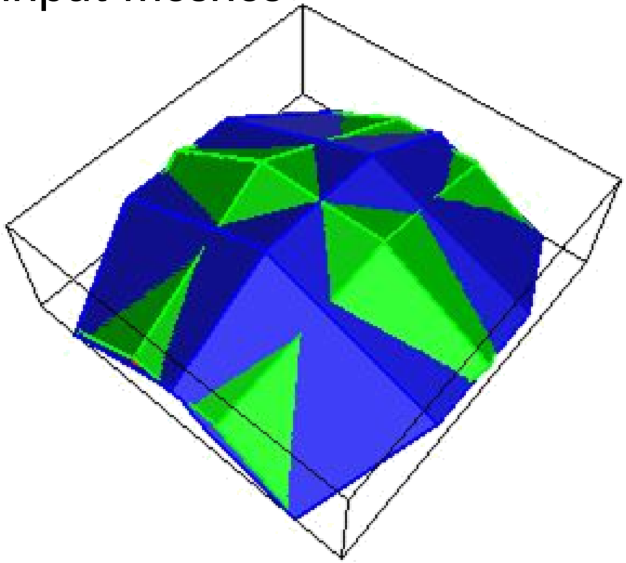
- Exchange interface data between meshes
  - Accurate and conservative methods
  - Scalable parallel implementation
- Common refinement of interface meshes
  - Interface has two different discretizations
  - Computes “intersections” of cells of input meshes



Quad. fluid surface



Tri. solid surface

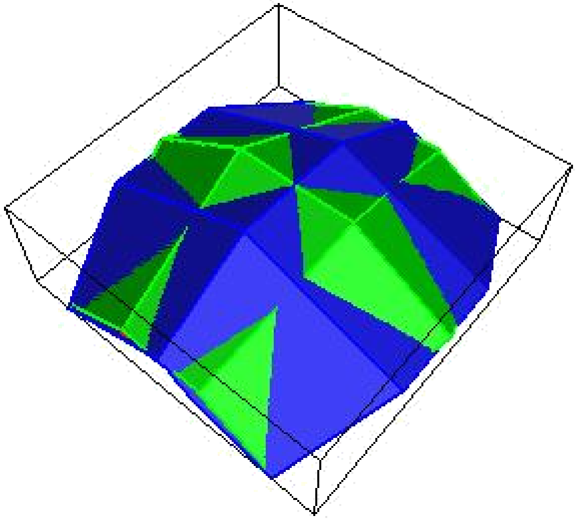


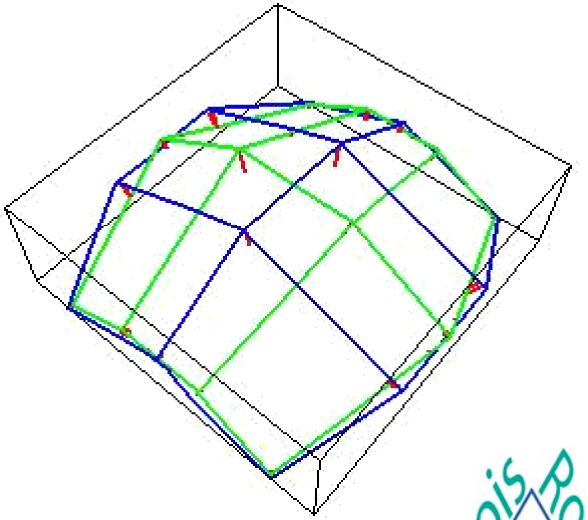
Non-matching meshes

Jiao X., and Heath, M.T., 2004, Common-refinement-based Data Transfer Between Non-matching Meshes in Multiphysics Simulations, International Journal for Numerical Methods in Engineering, 61(14): 2402-2427.

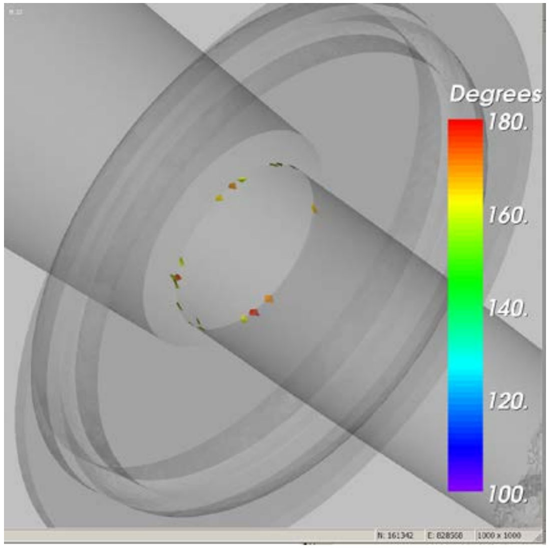
Interface Data Transfer: *Rocface 2.0*

- Interpolates quantities across non-matching meshes
- Constructs overlay mesh
  - Common refinement of two meshes
  - Enables exact mass and momentum conservation
- Minimizes errors
  - Coefficients provide smallest least squares norm
  - Huge (> 20x) improvement over standard method (Farhat, et al., 1995)

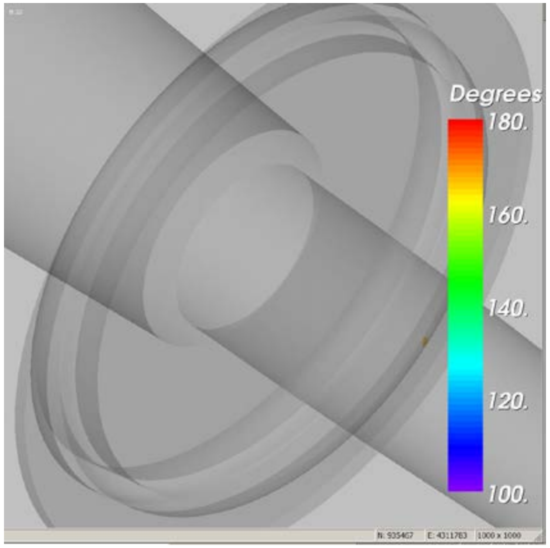




Mesh Enhancement Services



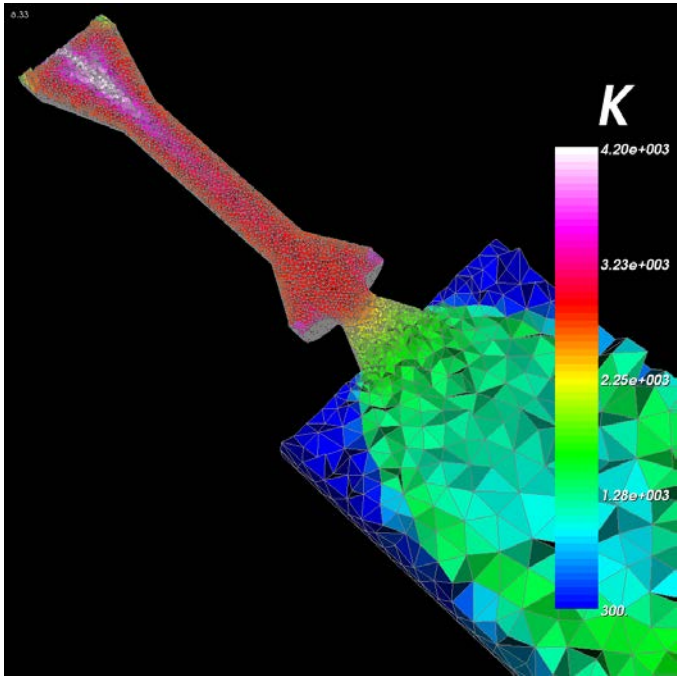
Bad elements eliminated

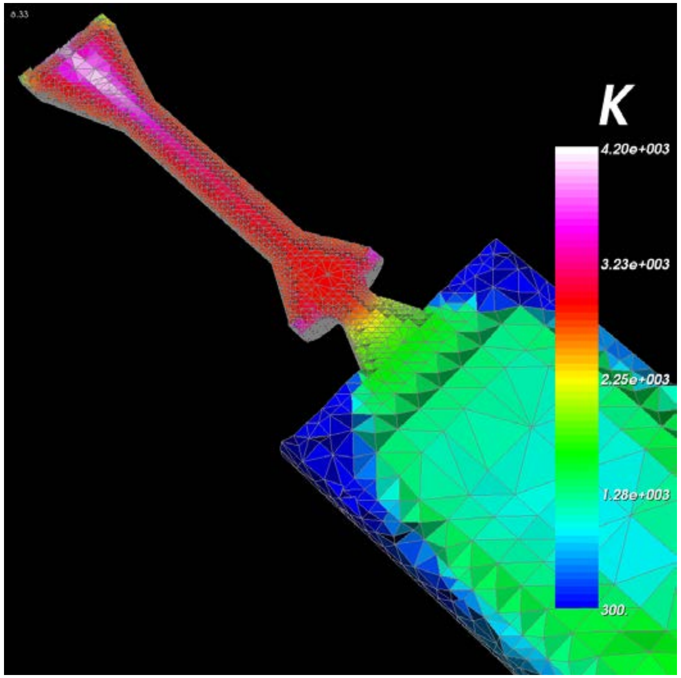


- Problem: degradation of mesh quality
- Three tiered approach
  - Mesh smoothing
    - Frequent
    - Relatively cheap
    - Not effective forever
  - Local mesh repair
    - Last ditch effort to avoid drastic consequence
      - Solution degradation
      - Simulation failure
      - Expensive remeshing
    - More expensive – data structures rebuilt
  - Global remeshing
    - Last resort – produce a whole new mesh
    - Most expensive
      - Time
      - Computational intensity
      - Simulation impact (fidelity)

Mesh Modification

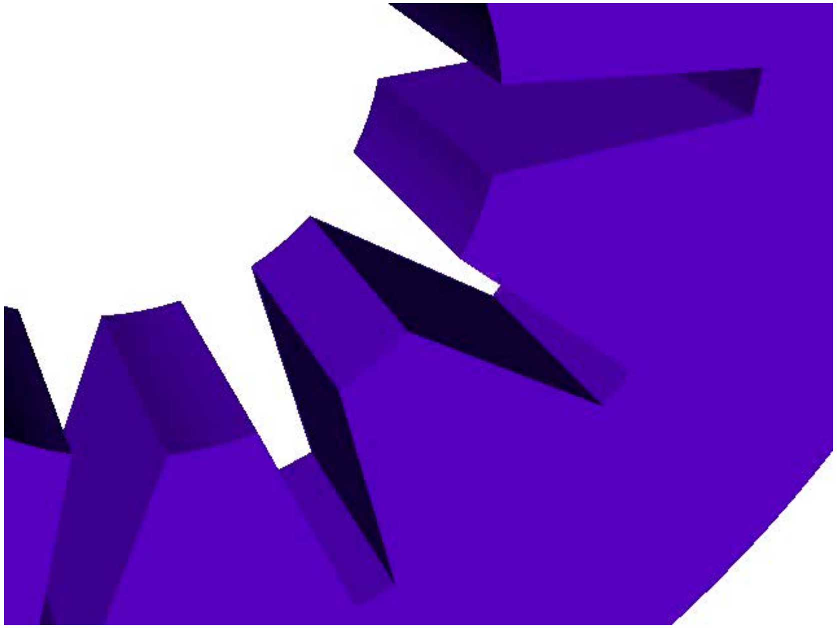
- Smoothing (frequent)
  - Uses parallelized version of MESQUITE (Sandia)
    - Reduce/average on shared nodes
  - Move existing nodes
  - No solution transfer required
- Local repair
  - Simmetrix driven
  - Modify existing mesh with basic operations
- Global remeshing (triggered)
  - Simmetrix driven
  - Produce new mesh of advanced geometry
  - General procedure:
    - Stitch together physical boundaries
    - Recreate geometrical model
      - Preserve features (unless too small)
    - Remesh surface
    - Remesh volume
    - Repartition for parallel execution
    - Transfer solution to new volume mesh
      - Volume weighted, conservative
    - Restart simulation



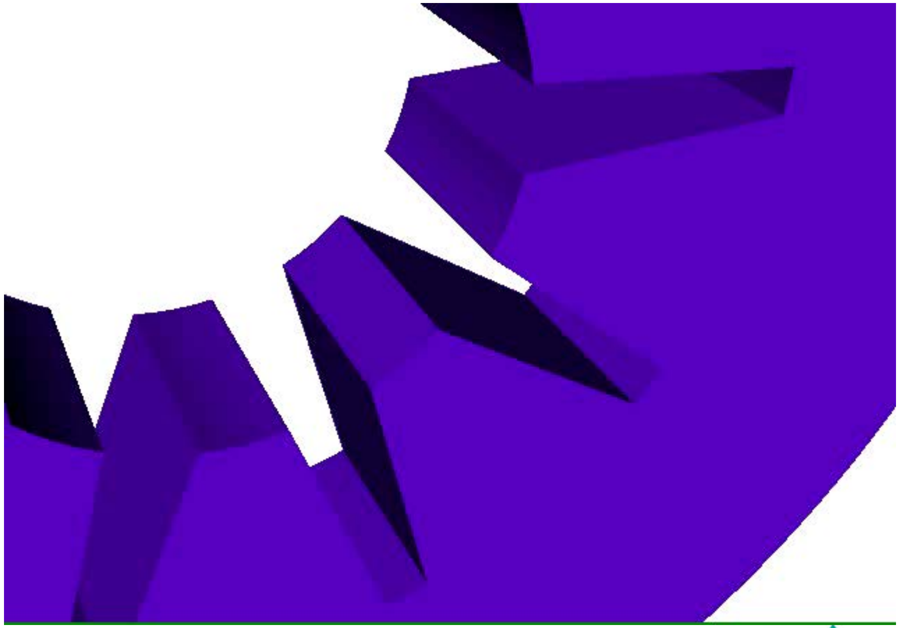


Dynamic Moving Interfaces

- Entropy-conserving surface propagation: face offsetting
- Moves vertices by constrained minimization
- Prevents development of cusps
- Redistributes vertices in tangent space



Marker-particle method

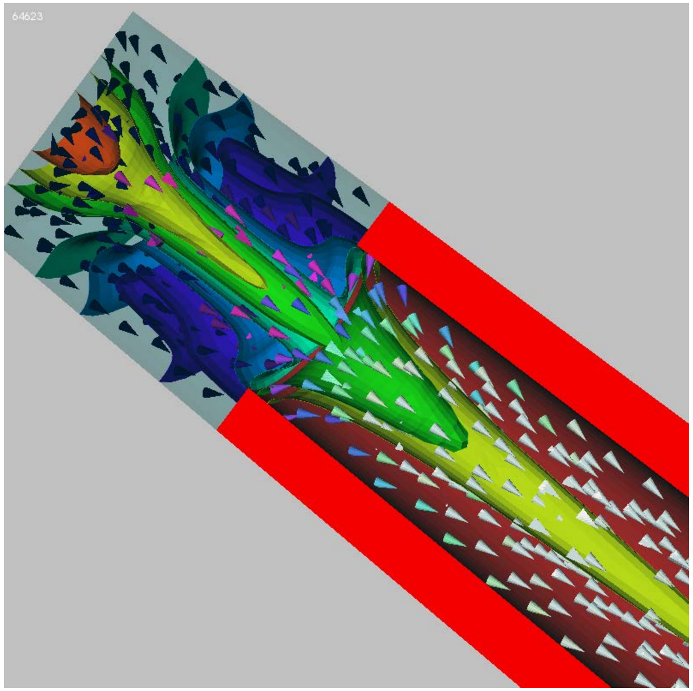


Face-offsetting method

Infrastructure Summary

- Software integration infrastructure
  - Facilitates integration of independently developed codes (MPI Libraries)
  - Publication of native methods and data structures
  - High-level data management
  - Requires few changes to existing apps
  - Encapsulation into component objects called modules
  - OO oriented module management

- Service modules
  - High-level middleware utilities
  - State-of-the-art numerical and geometric algorithms
  - Advanced novel data mapping



- High-level orchestration infrastructure
  - Designed to accommodate growing complexities
  - Static interface for physics modules
    - Plug and play
  - High-level Simulation API
  - Work in progress