Loci: Logic Programming for Computational Field Simulations

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Motivation

- Complexity of numerical simulation software is increasing
- Current state-of-the-art with respect to parallel computing is labor intensive and prone to errors
- Concerns of reliability and rapid prototyping are important to domains where efficient means of modeling are unknown

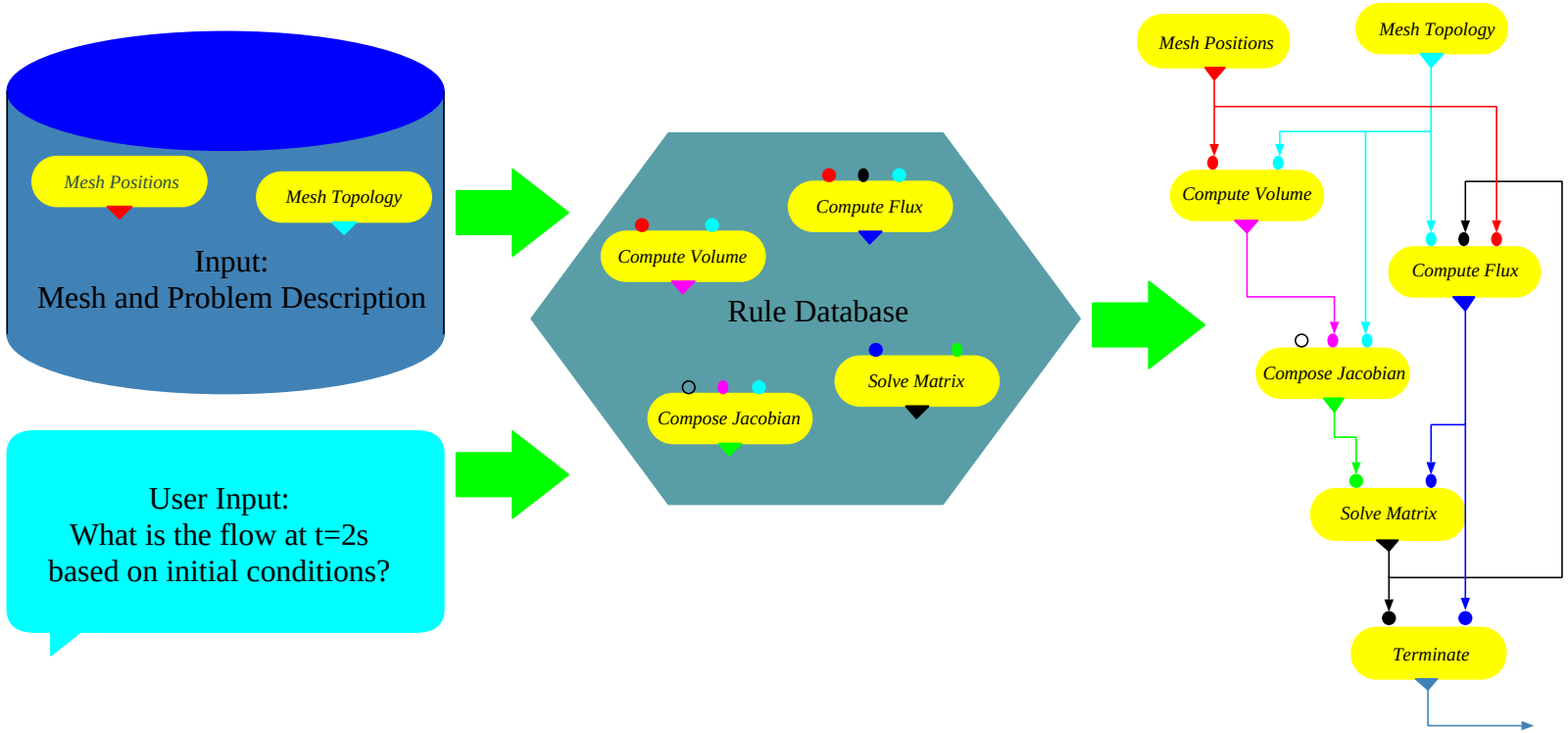
Key Concepts

- Computations are performed with respect to numerical discretizations called meshes.
- Meshes can be represented as a collection of entities combined with a set of binary relations called maps.
- Computations are performed by binding values to entities.
- Many computations are based on values assigned to neighboring entities. The binary relations used to represent the mesh are invoked in the access of these neighboring entities.

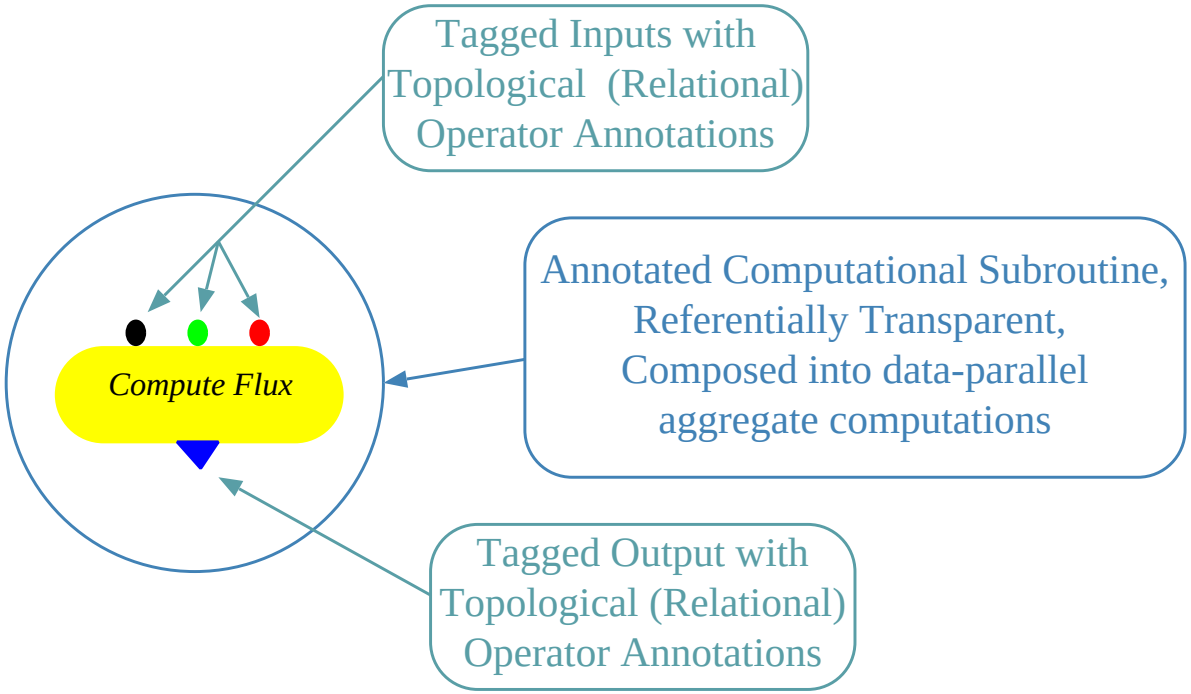
Key Observations

- Entities can generally be partitioned into a set of entities categories. The number of these categories are relatively independent of grid density.
- Since values tend to bind to entities according to category, pre-sorting entities by category facilitates $O(1)$ computation of set intersections, unions, and complements.
- Many computations are of a declarative nature. For example: In an ideal gas, pressure is calculated using density and temperature.
- Simple and compose-able components facilitate reuse.

Paradigm: Programming by Rule Database



Rules Represent Annotations to Stateless Subroutines



A Simple Example

Consider the ideal gas law for mixtures of thermally perfect gases:

$$p = \rho \tilde{R} T$$

This equation establishes a relationship of pressure to density, temperature, and mixture gas constant. This relationship is universal: it applies to any place where these properties are simultaneously available at any instant in time.

A Simple Example (cont)

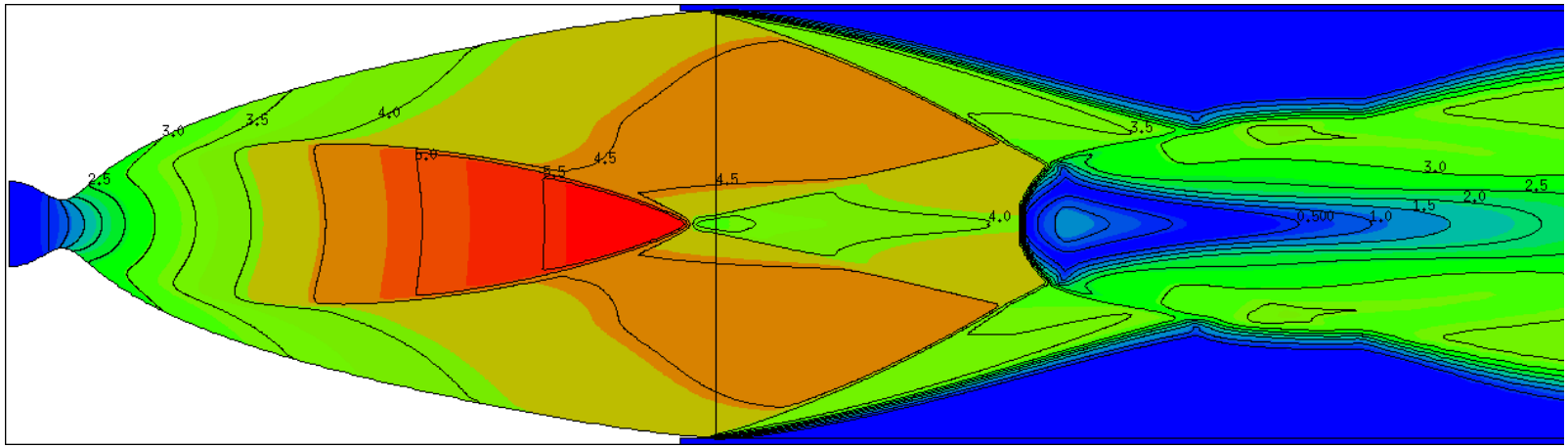
The ideal gas law relation can be represented by the rule signature

$$p \leftarrow \rho, \tilde{R}, T$$

This rule signature signifies that a value for pressure can be generated from values for density, temperature, and mixture gas constant. It is described by the implication:

$$value(\rho) \wedge value(\tilde{R}) \wedge value(T) \Rightarrow value(p)$$

An Overview of the Chem Code

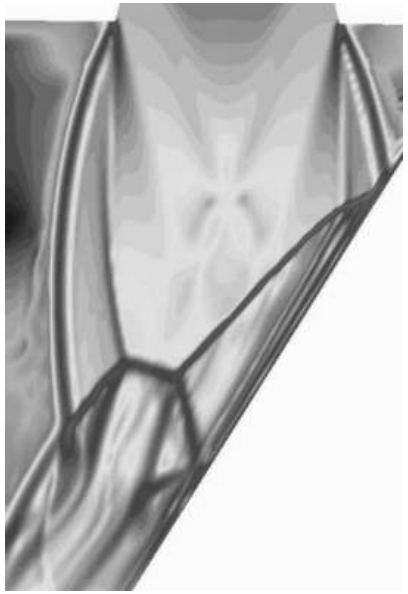


- General reaction kinetics, thermodynamic, and transport models
- High-Resolution Approximate Riemann Solvers
- Fully implicit, time-accurate and steady-state formulation
- Explicit Runge-Kutta integration formulation also supported
- Support for Generalized Grids (arbitrary polyhedra)
- 4th order MacCormack integration method supported for LES

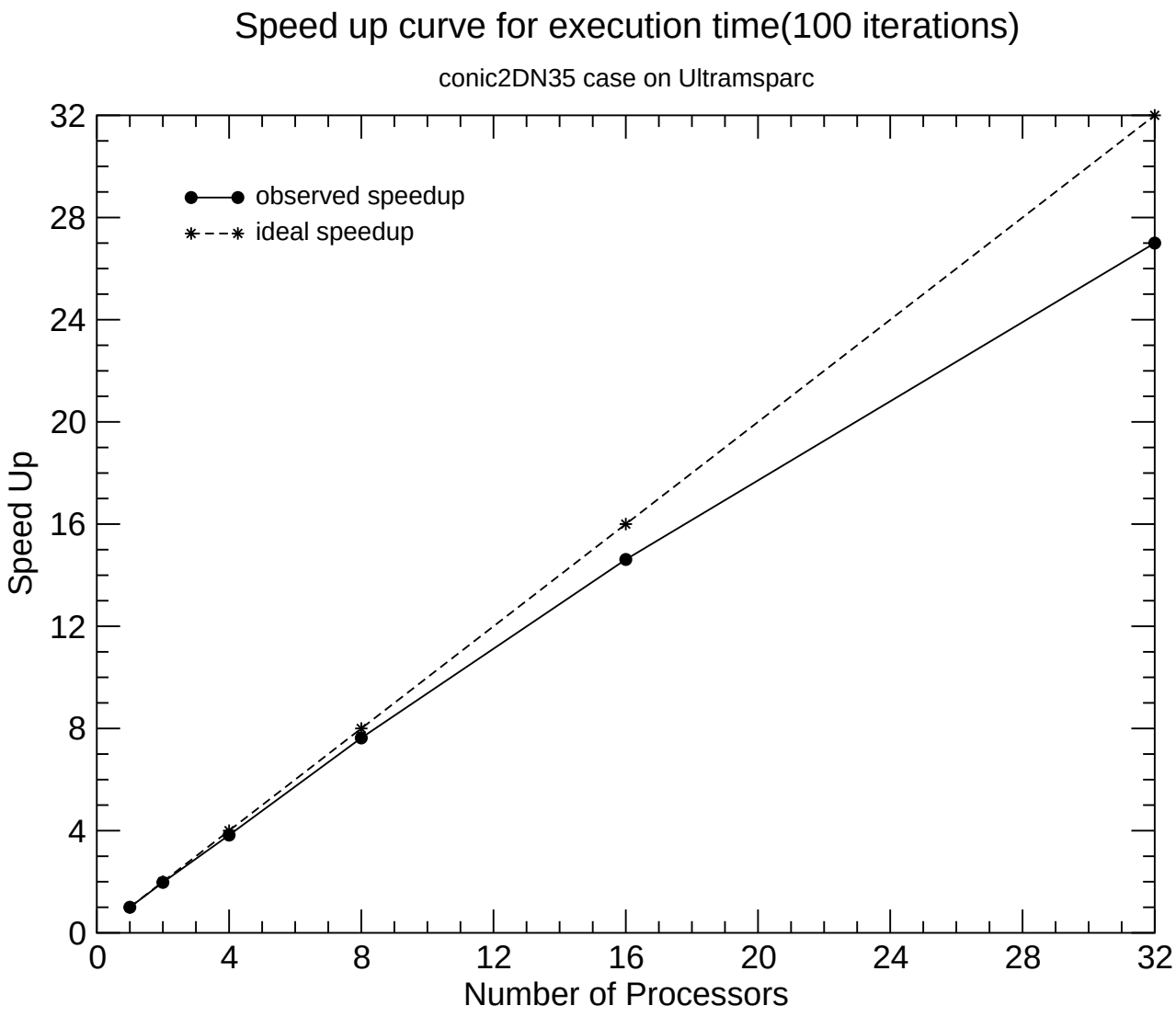
Parallel Implementation

- Uses both MPI and POSIX-threads.
- Parallelization is automatic (No parallel directives are used in model specifications.)
- Parallelization supports arbitrary decompositions of entities.
- Future work will include dynamic load balancing both in the POSIX thread model and MPI.

Performance Benchmark



- Test case is a 3D inviscid non-reacting supersonic jet impingement problem.
- 600K cells in a structured multiblock grid.


Speed up curve for execution time(100 iterations)
conic2DN35 case on Ultramsparc
observed speedup
ideal speedup
Speed Up
Number of Processors
0
4
8
12
16
20
24
28
32

Coupling Fluids and Solid Mechanics using Loci

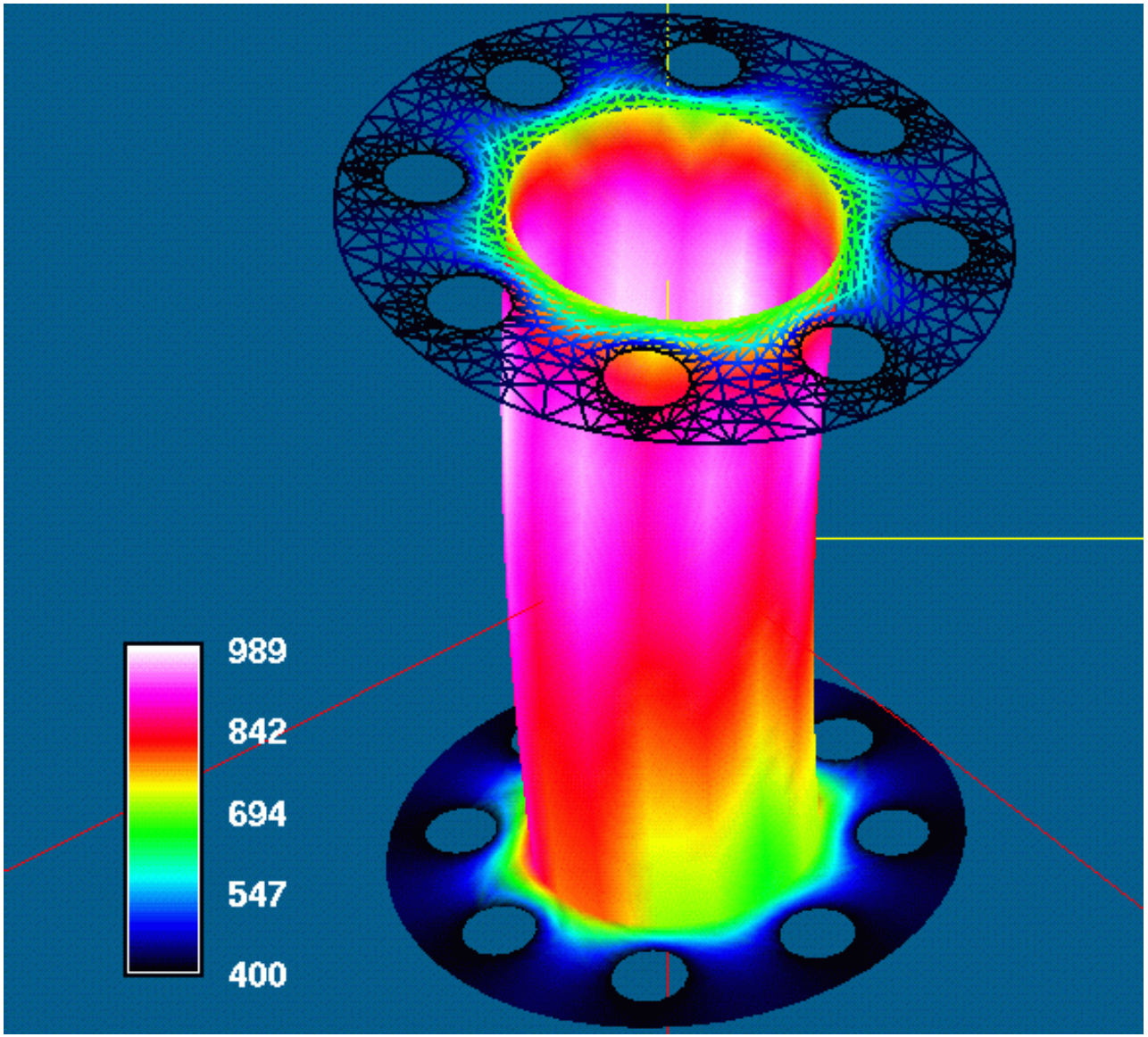
Fracture and Fluid Mechanics

- Gas under high temperature and Pressure such as encountered in propulsion systems and high efficiency steam turbines.
- Concern: Failure of containment of these gases
- Fracture mechanics problems dominated by thermal and mechanical loads due to above gases. It is a multidisciplinary problem.
- MSU - Gas Phase Models
- Cornell - Fracture Mechanics Models

Model Problem

- Regeneratively Cooled curved pipe (Idealized Problem)
- Gas Phase: Chem Code provides model
- Solid Phase: FEM model for aniostropic non-linear thermal and mechanical response. (Under development at Cornell)

Unsteady thermal response at 10ms



Loci for MD Topics

- Loci is a research tool that is currently under development
- Focused on Fine-Grained inter-operation of 3D models for time accurate MD simulations.
- Not constrained to 3D
- Coupling to external codes planned for next year.
- Provides automatic parallelization
- Ported to Unix and Linux Systems (SGI, Sun, x86)