Encore: A Toolkit for Verification, Postprocessing, Error Estimation and Adaptivity

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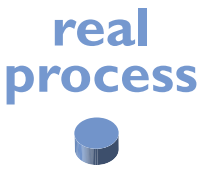
Sandia National Laboratories

ADVANCED SIMULATION & COMPUTING™

Outline

Errors and Uncertainties



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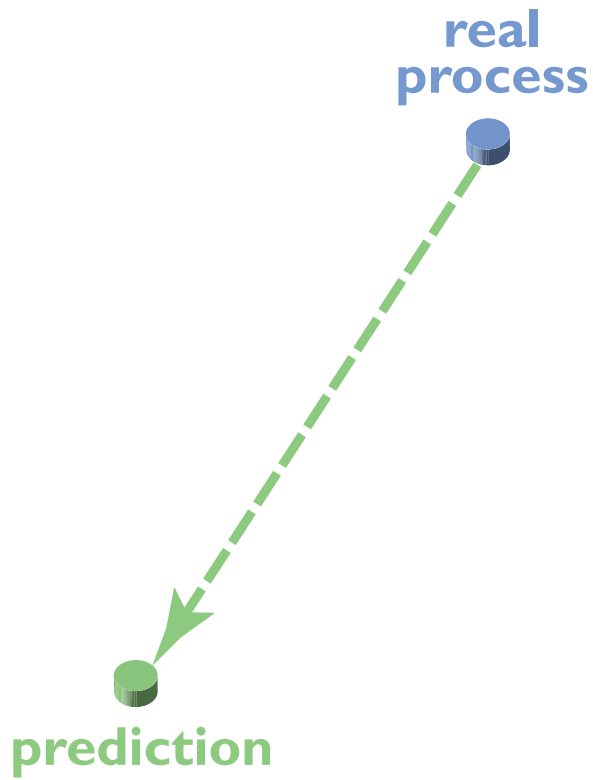

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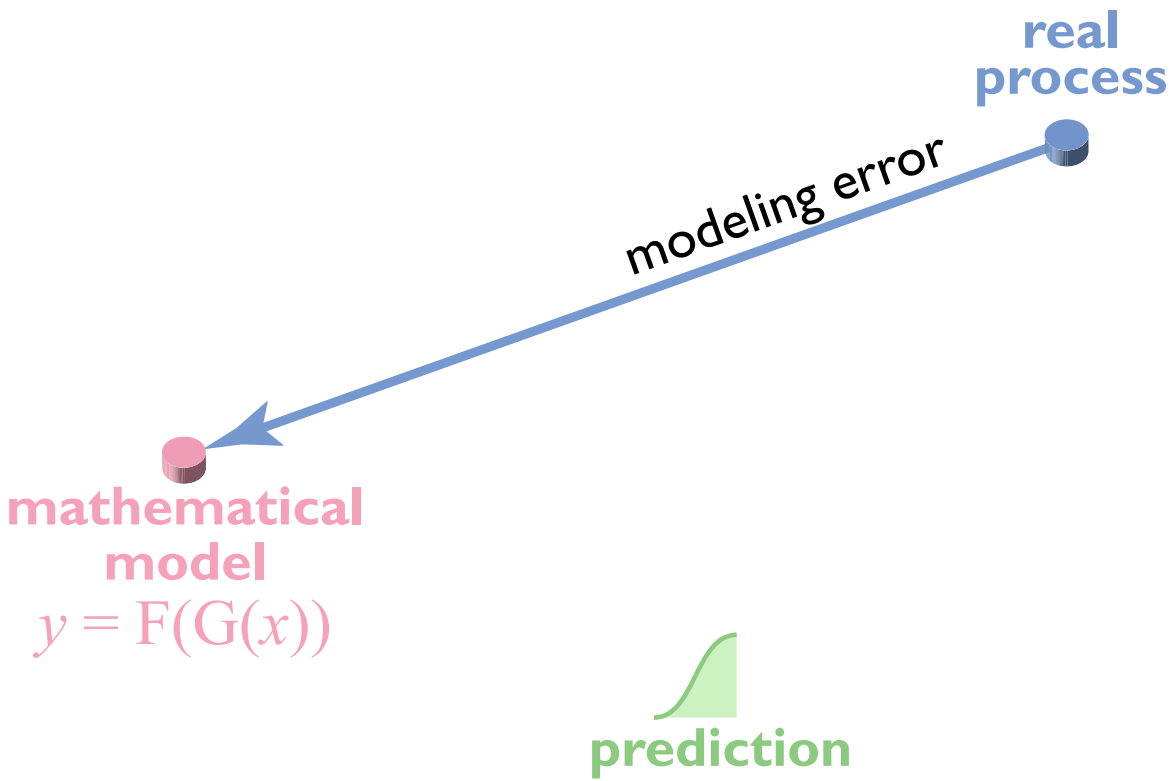

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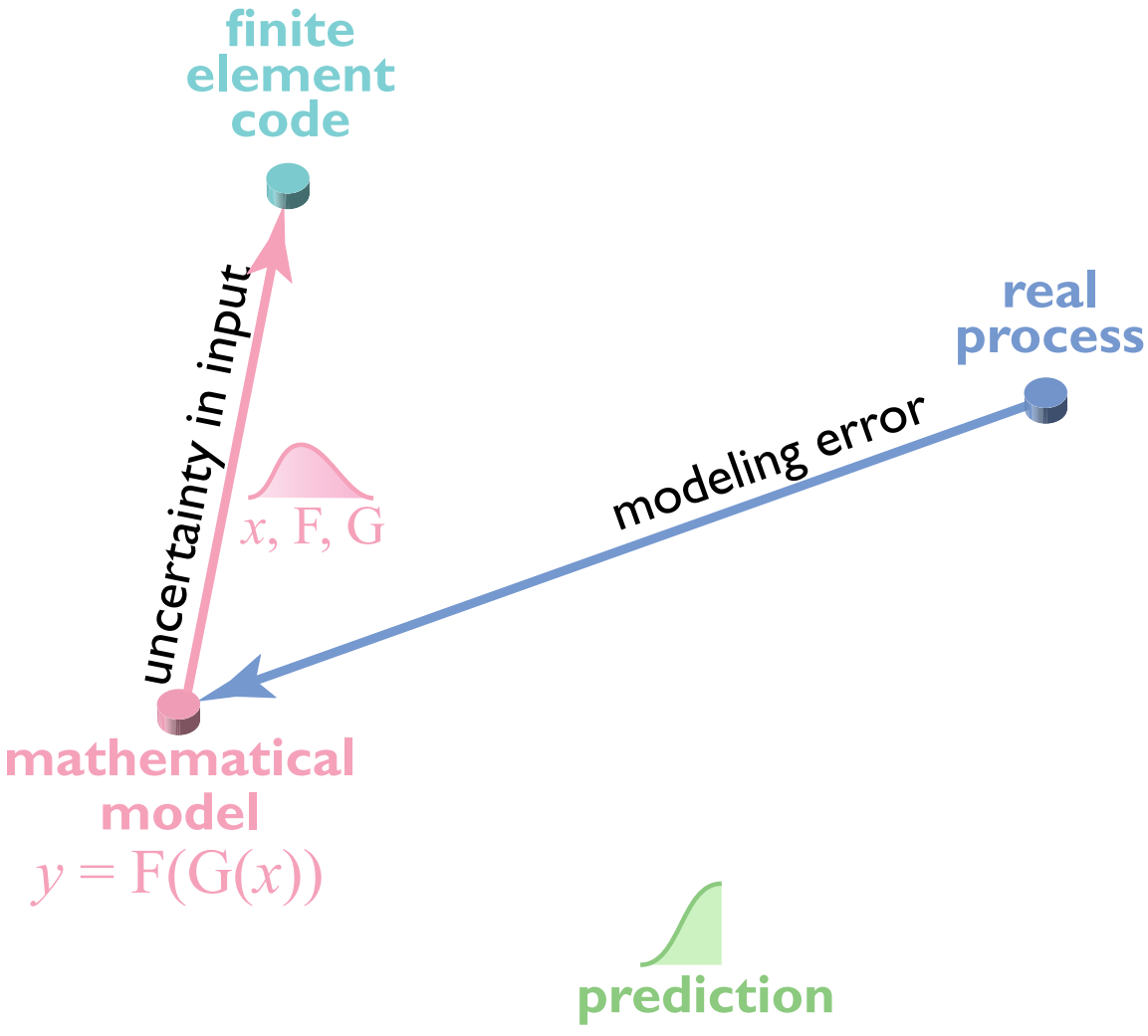

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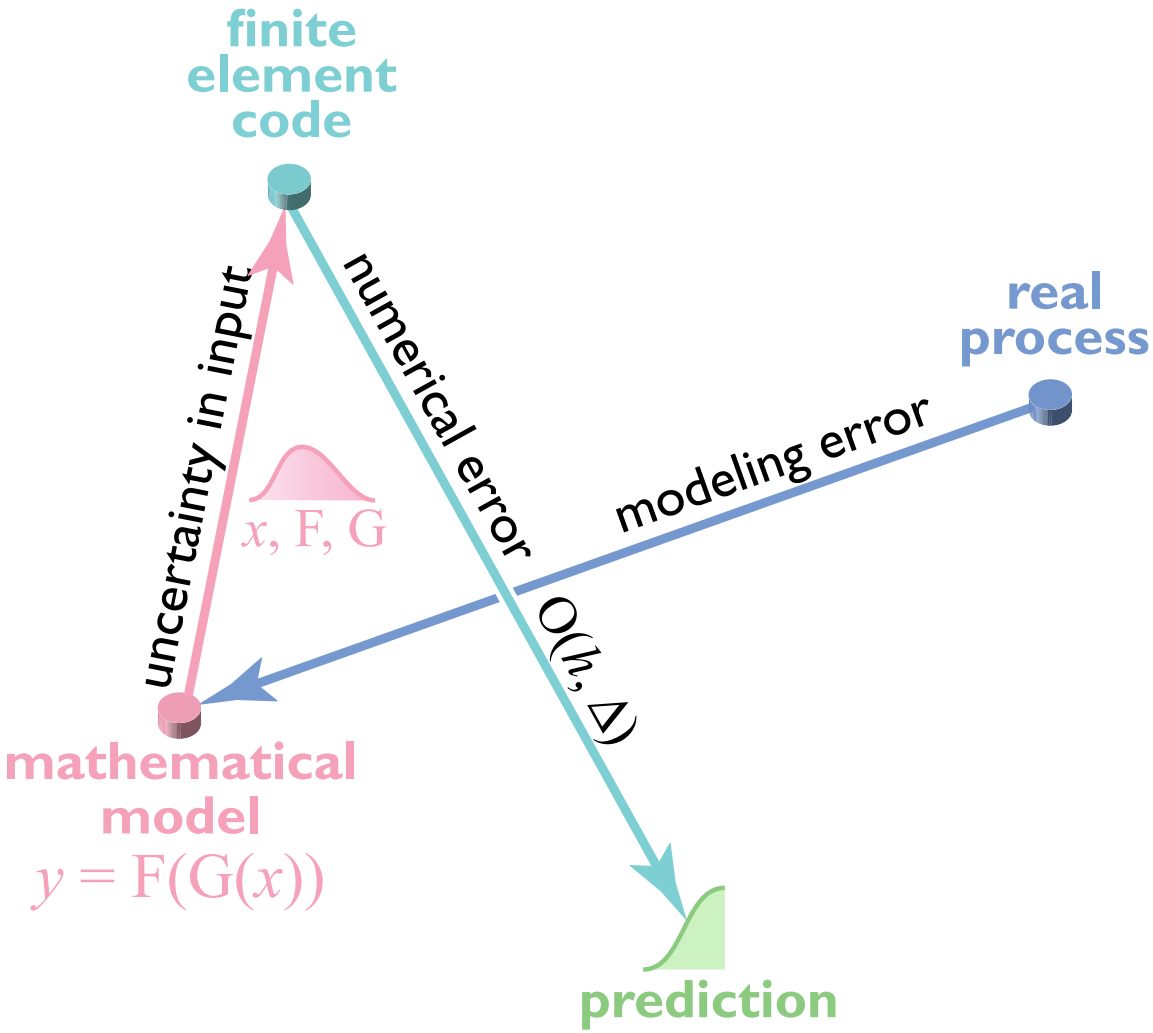

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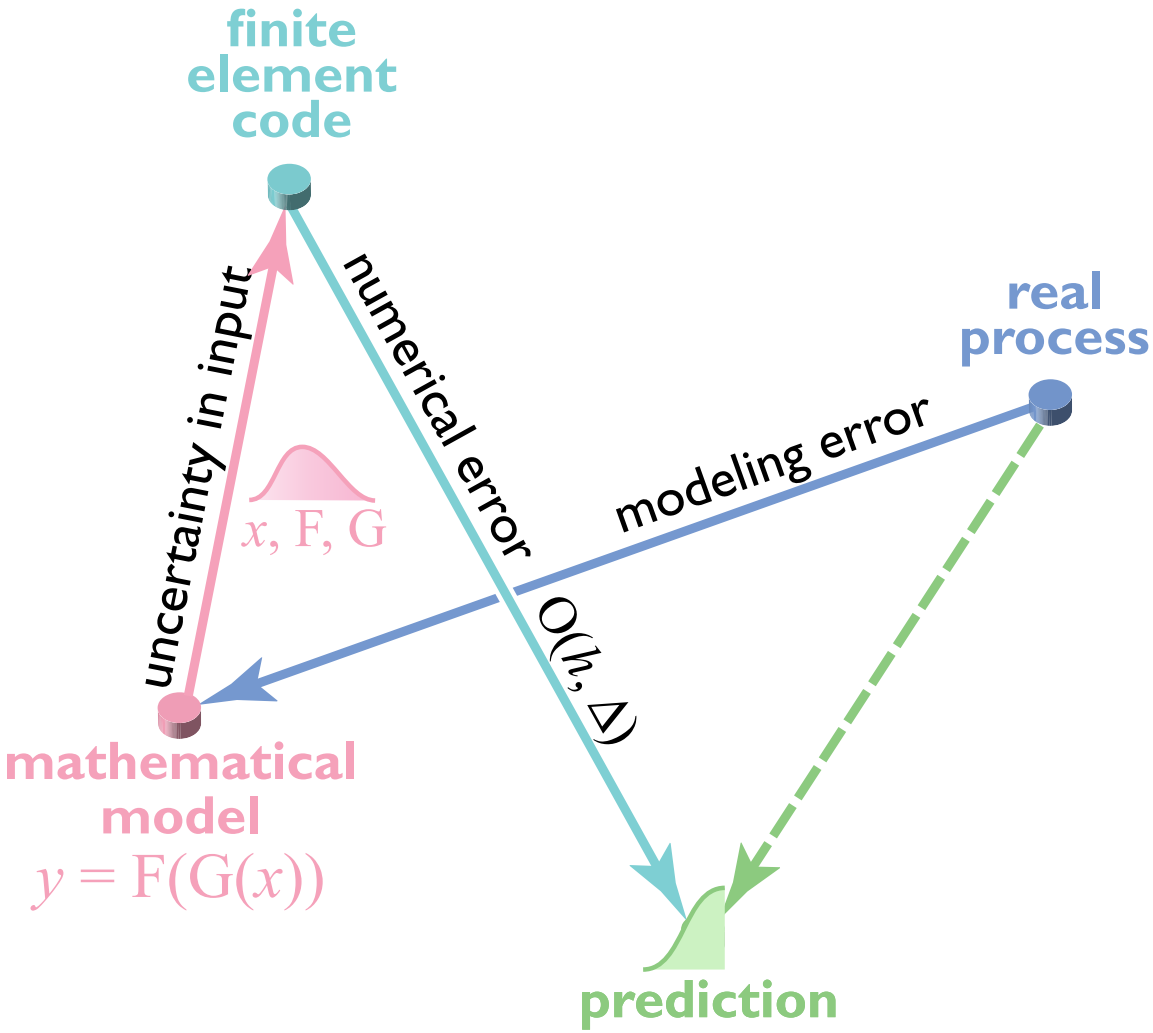

Strategic Goals of Encore

Enable **predictive** simulation

- Unified, modular services for code and solution verification.
- Manage tradeoff of resources versus accuracy.
- Make it easy for users and developers to provide extensions.
- Bridge between ASC codes and UQ tools (Dakota, Trilinos).

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Encore Features

- Code/Solution Verification
  - Facilities for generating and driving manufactured solutions.
  - Comparison between two simulations or simulation and analytic.
  - Tools for order of accuracy verification and extrapolation.
- Postprocessing
  - Calculating derived (response, observable) quantities.
  - Extendable through simple user subroutine capability.
- Error Estimation
  - Suite of physics independent error indicators.
  - Support for physics dependent error estimation. (Adjoint, etc.)
- Adaptivity
  - New flexible, user driven adaptive system.
  - Markers based on features or error.
  - Consolidation of Sierra adaptivity infrastructure.

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- Version 1.0 released Oct. 2007
  Presentation Nov. 5th, 2007
  Hands-On training Dec. 6th, 2007
- Funded in part by ASC Algorithms and V&V Program.
- Software Quality Data:
  - Trackers Submitted: 233 Closed: 152
  - Lines of Code: 30,000 (about 1/3 of **Calore**)
  - Regression Tests: Over 120
    75% Line Coverage
- Online library linked with any Sierra Mechanics application.
  Currently **Adagio**, **Aria** and **Calore**.
- Off-line stand-alone executable.
  Physics independent, read and write Exodus files.

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Leveraging SIERRA Mechanics Technology

- Can be run from any Sierra Mechanics supported platform.
- **Encore** output is either Exodus file(s) or tabular data.
  No graphical output.
- Ability to process application's runtime data.
- SIERRA Framework Features used by **Encore**:
  - Parallel load balancing
  - Distributed I/O database
  - Element library (2D and 3D, unstructured grids)
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part 1

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- Function Interface
- Postprocessors
  - Evaluation
  - Norms
  - Integrals
  - Import/Create
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  - Patch Recovery
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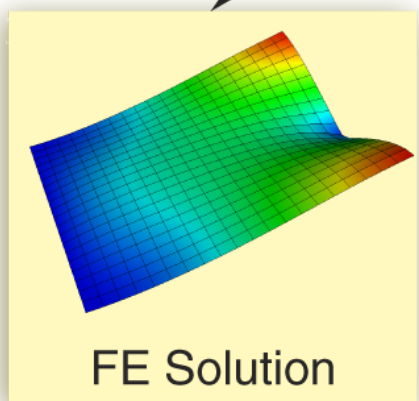

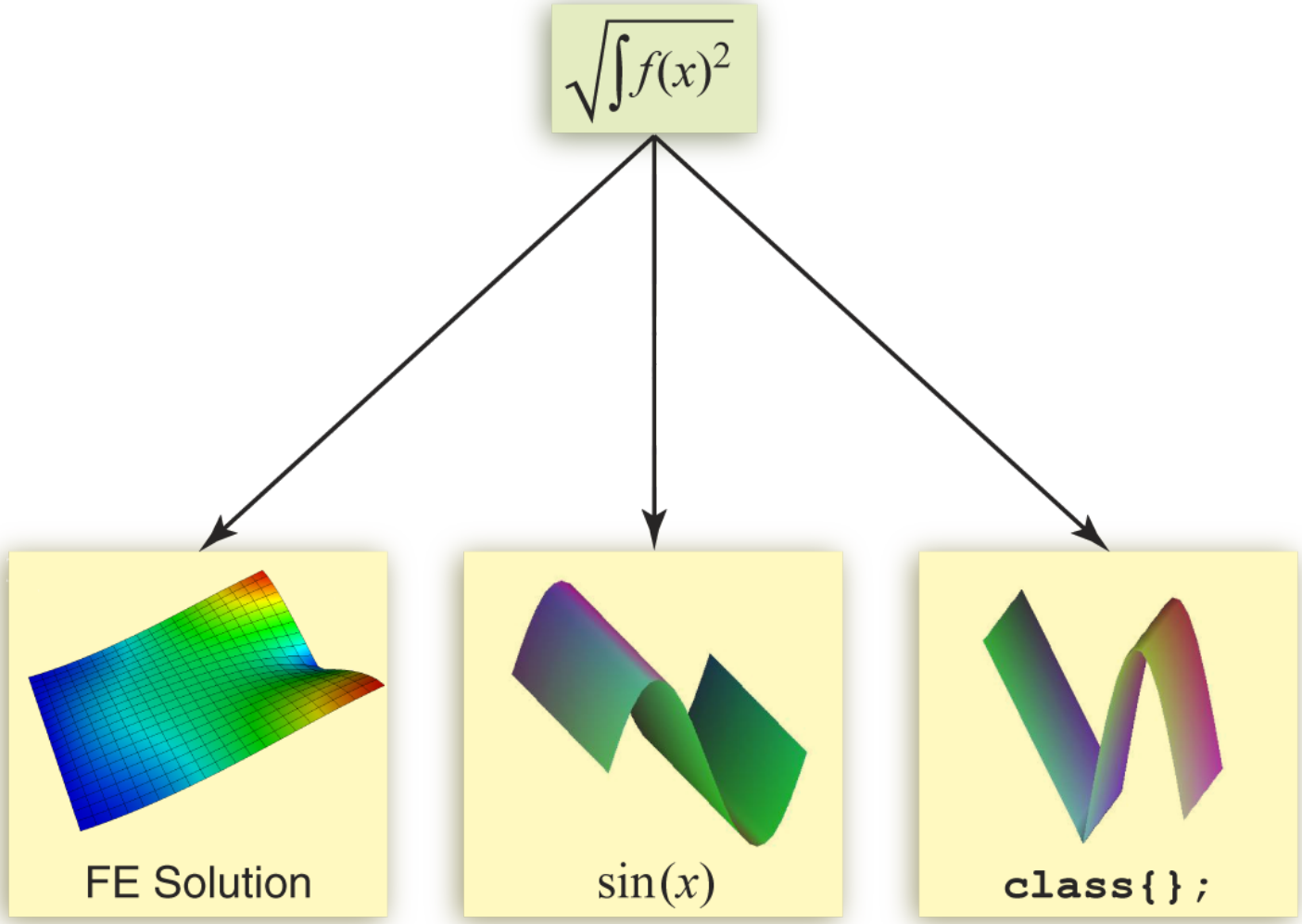
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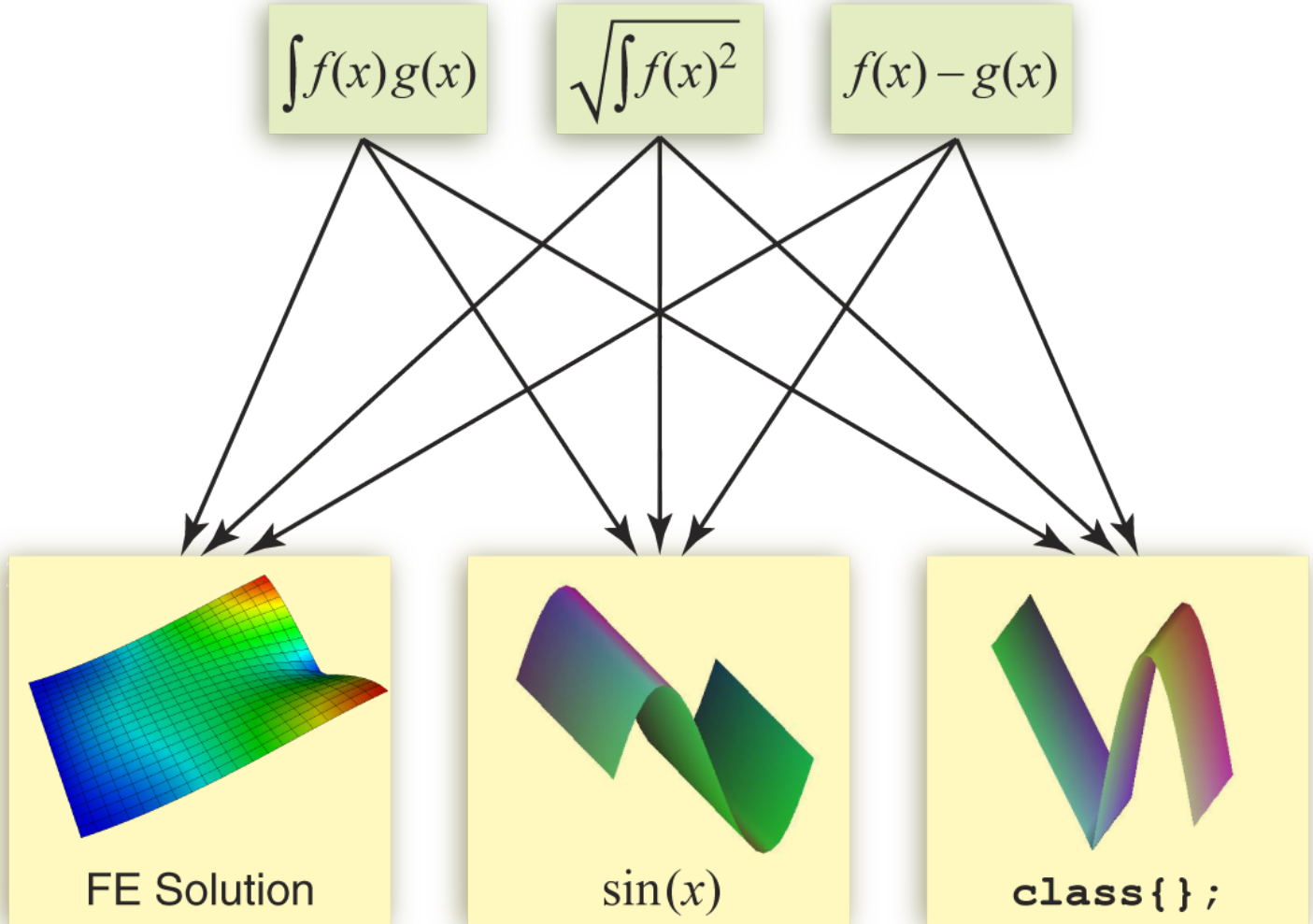
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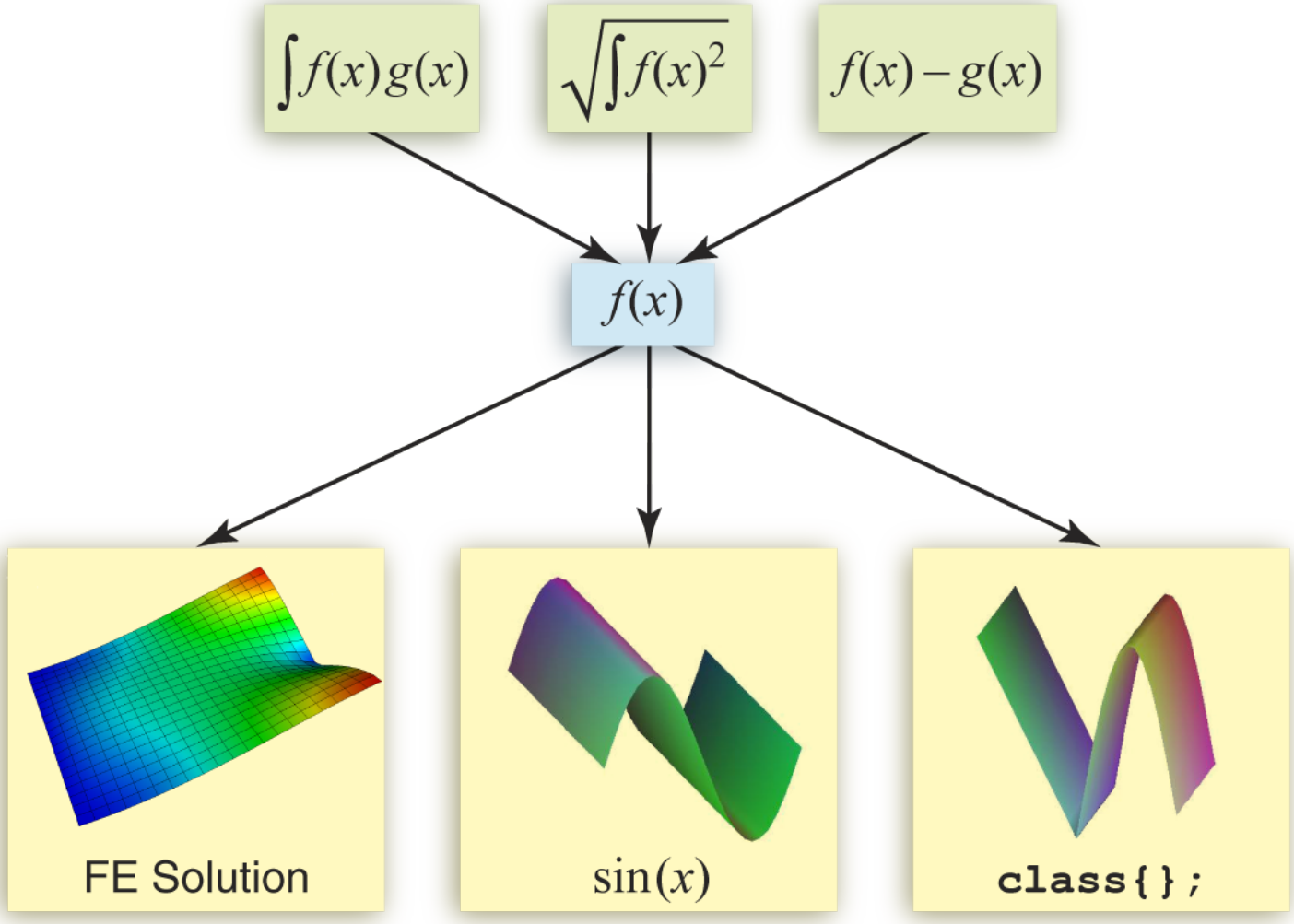
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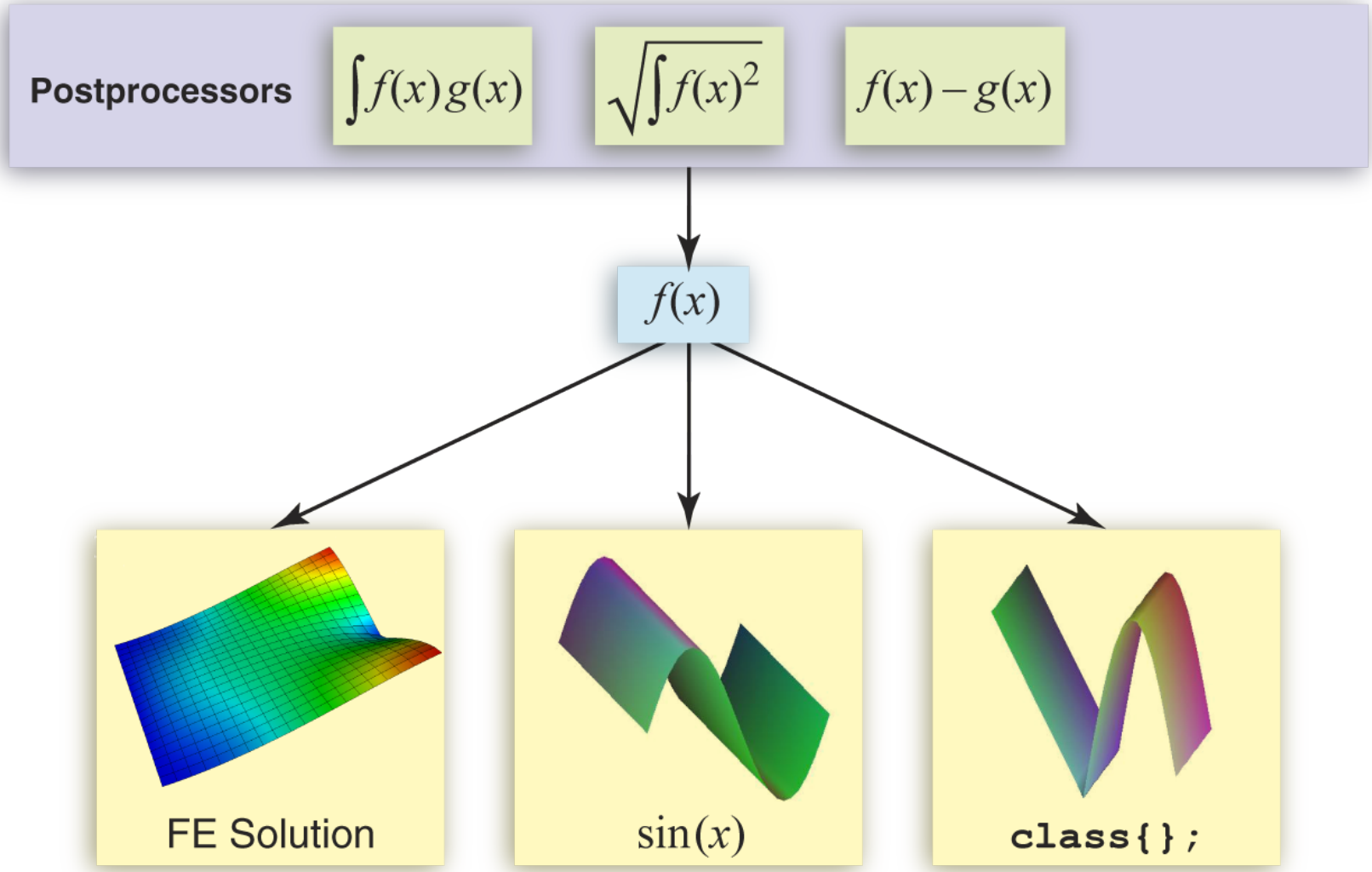
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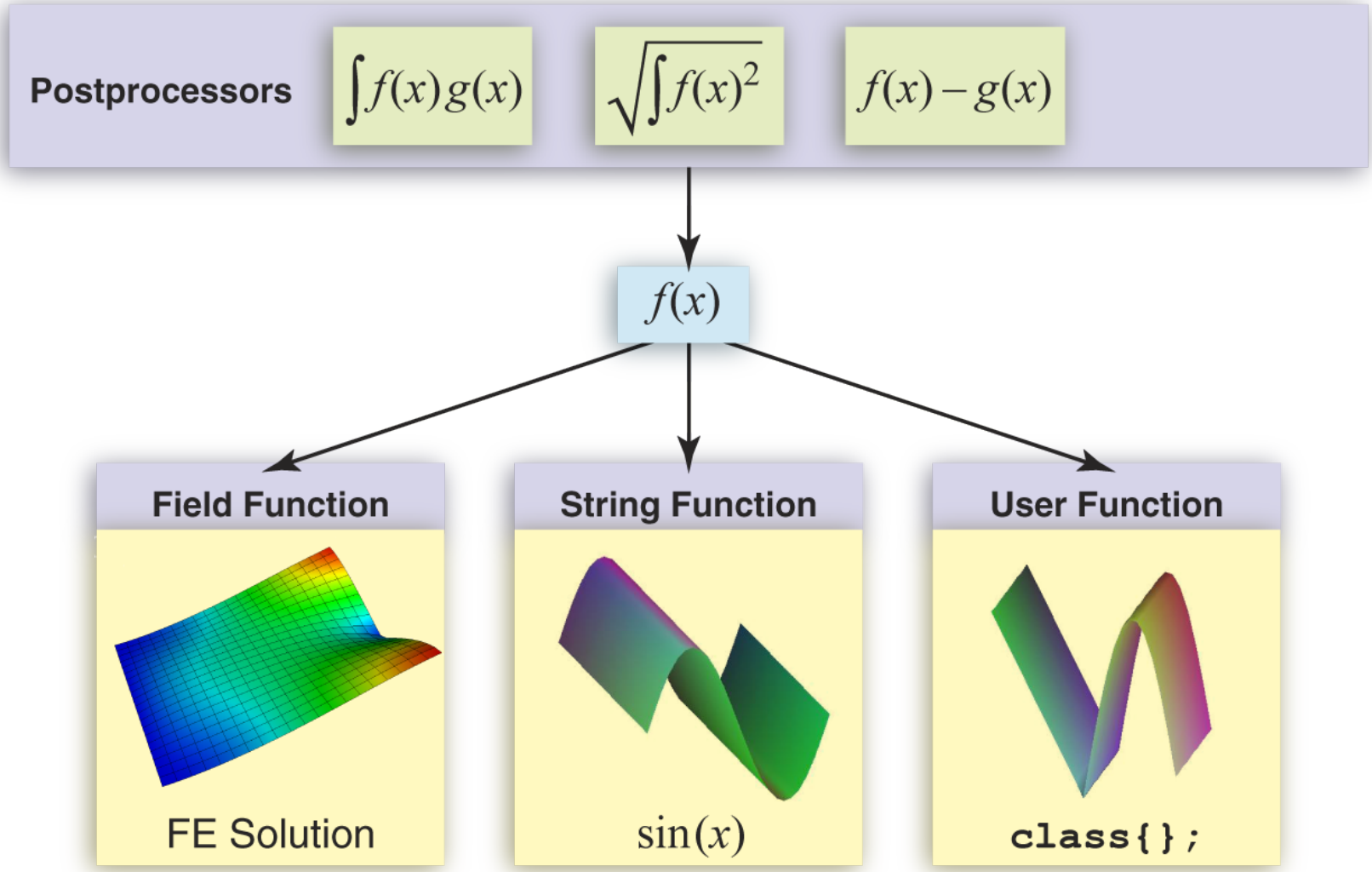
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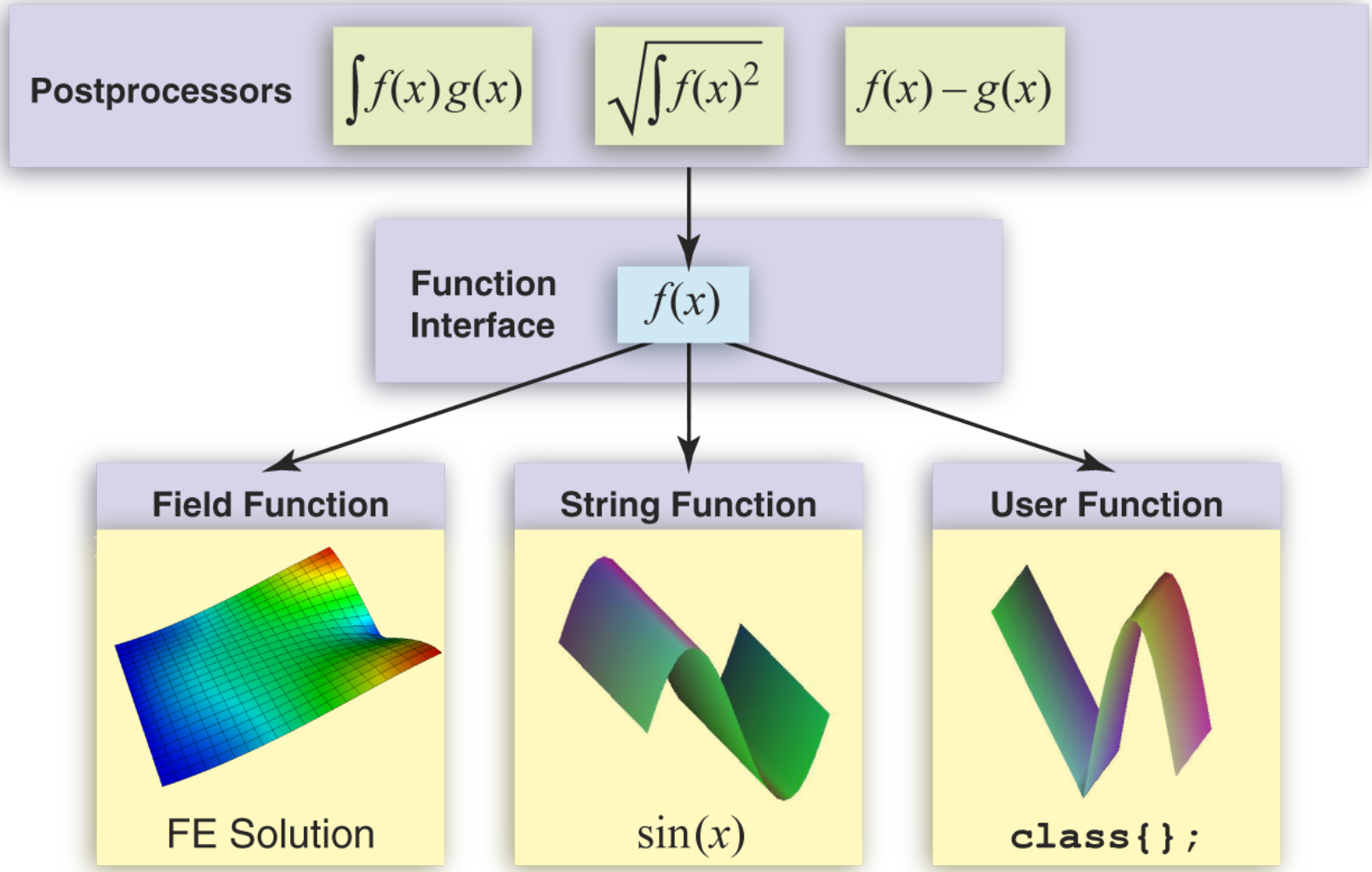
Postprocessors
$\int f(x)g(x)$
$\sqrt{\int f(x)^2}$
$f(x)-g(x)$
Function Interface
$f(x)$
Field Function
FE Solution
String Function
$\sin(x)$
User Function
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Function—abstract interface

$f(x)$

- Users do not need to know implementation details.
- Functions can represent analytic expressions or simulation results.
- Users can mix and match types of functions.
- Functions can be scalar/vector/tensor valued.
- All types of functions provide:
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Types of Functions

- A **Field Function** represents simulation fields on a mesh.
- **String Functions** are analytic expressions that users type in an input file.
  - For example: "`x + a * sin(y)`".
- **User Functions** are C++ code that users write, allowing piecewise defined values and series solutions. They are dynamically linked into a SIERRA Mechanics applications—fast and easy.
- Function combinations: **Difference Function**, **Product Function**.
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$$error = u(\mathbf{x}, t) - u_h(\mathbf{x}, t)$$

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Postprocessors

- Postprocessors (PPs) are calculations that run:
  - After initial conditions,
  - After a non-linear step,
  - After every timestep,
  - At a certain simulation time.
- Input to most PPs are Functions.
- Output of PPs are
  - Simulation fields (on nodes, elements, etc.)
  - Formatted tables in a text file—for Excel/Matlab/etc.
- PPs are fully parallel.
- Can be easily extended by users.

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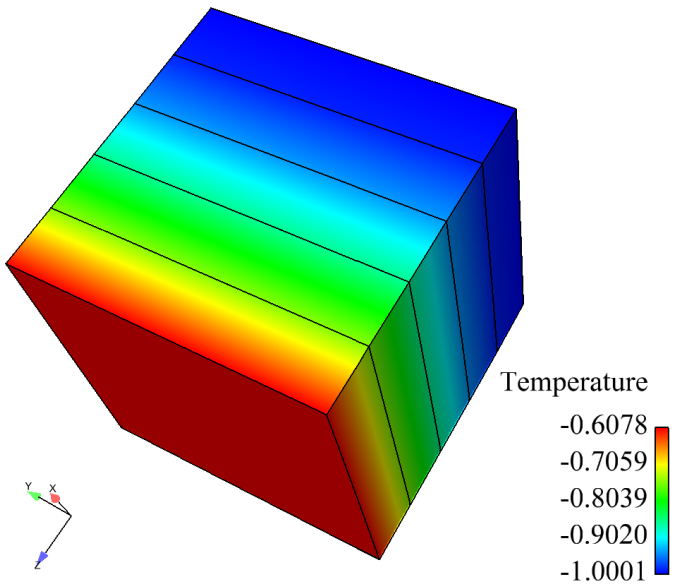
Evaluate Postprocessor

- In order to compare to experimental values, analysts need to probe simulation values.
- The **Evaluation PP** takes a Function and evaluates it at any point in space/time.
- Any type of evaluation (Value, Gradient, Time Derivative, Stress, Flux) can be performed on a function.
- In order to perform code verification, a user could evaluate the difference between the simulation and an analytic solution while the simulation is running.

Example: Evaluate the simulation field temperature at a point, $T(0, 0, 0)$

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encorereg Postprocessor Output for Group agroup
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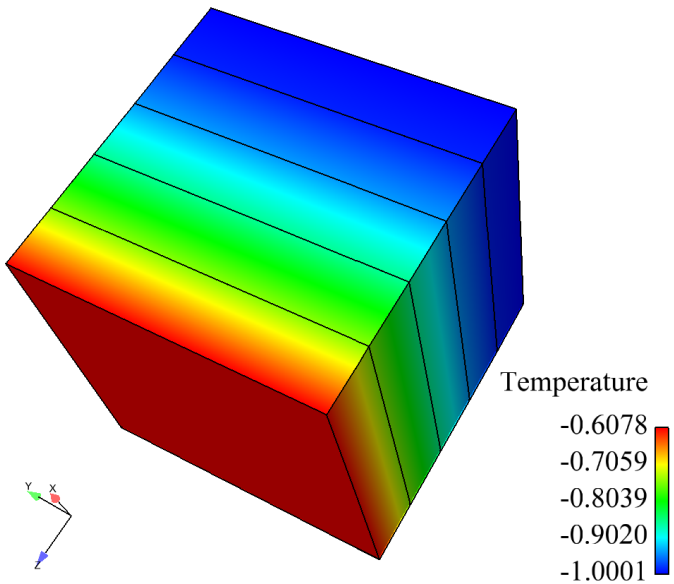


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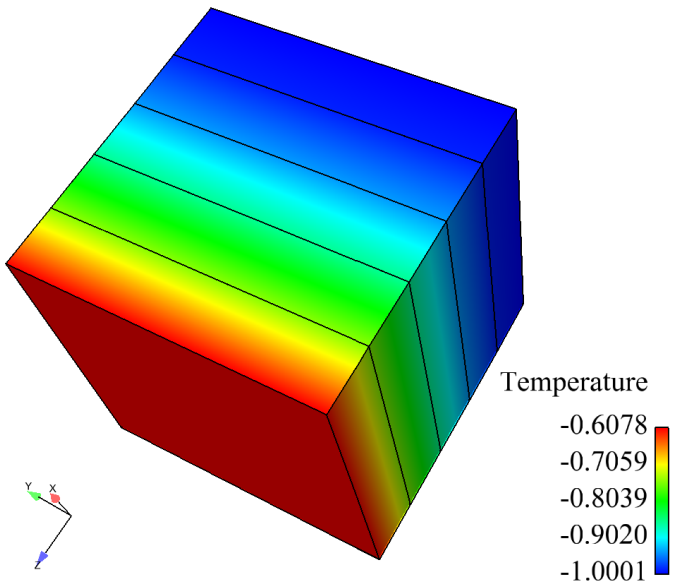


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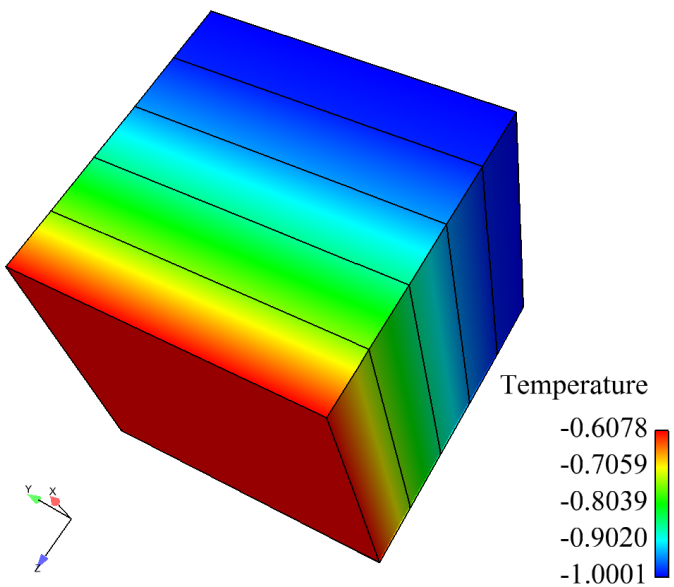


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- For code verification using order of convergence, accurate calculation of global norms is essential.
- Output of **Encore** Norms:
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- Common global norms in **Encore**:

$$||u||_{L^2(\Omega)} \equiv \left(\int_\Omega |u|^2 \, dx \right)^{\frac{1}{2}} \approx \left(\sum_{elem} \underbrace{\sum_q |u(x_q)|^2 \, |JxW|_q}_{\text{element contribution}} \right)^{\frac{1}{2}}$$

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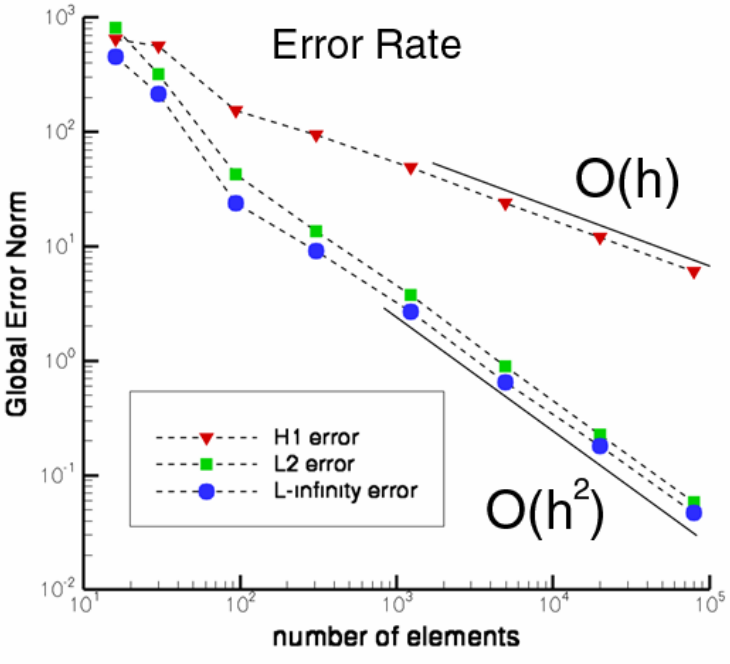
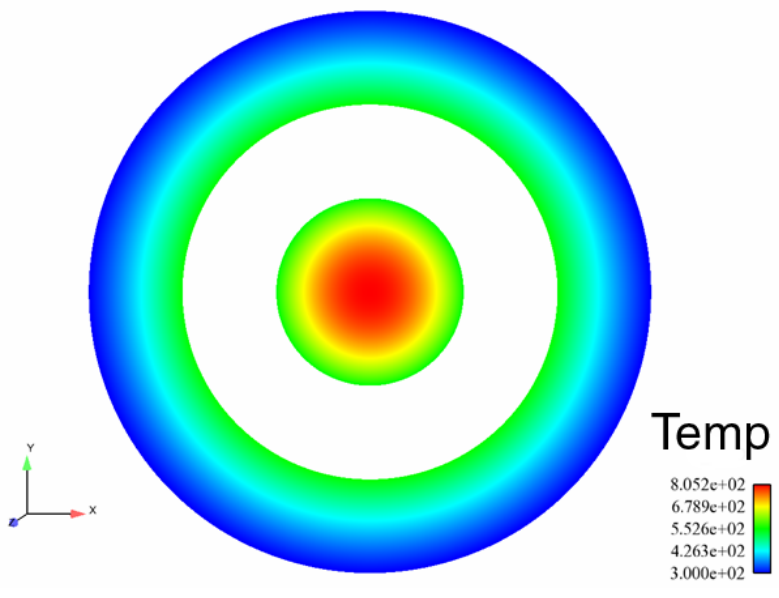
Example: Calore Verification

- These norms have been used in verification studies of **Calore** (FY07 Level 2 Tri-Lab Verification Milestone).
- Example: **Calore** coupled conduction/enclosure radiation problem.
- Using an exact analytic solution, the error in each global norm can be calculated, and the order of convergence verified.





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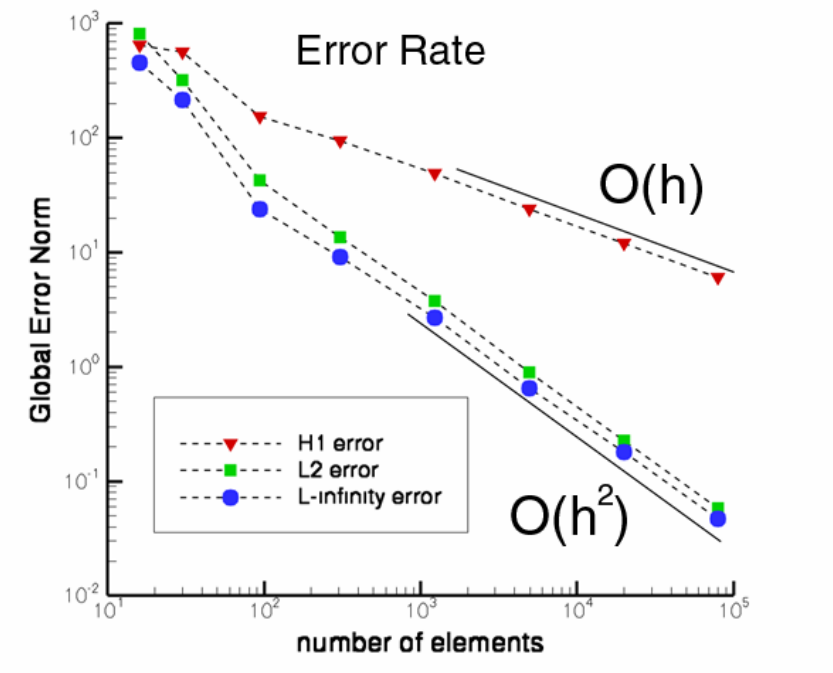

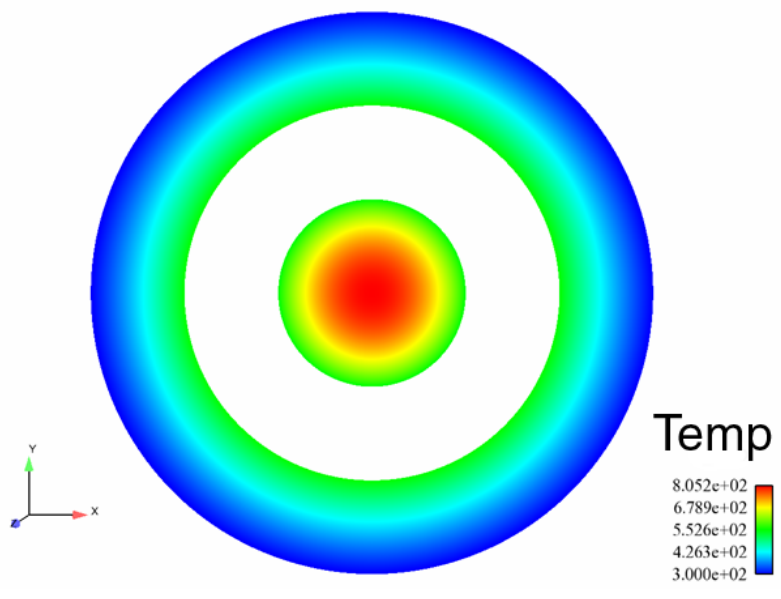

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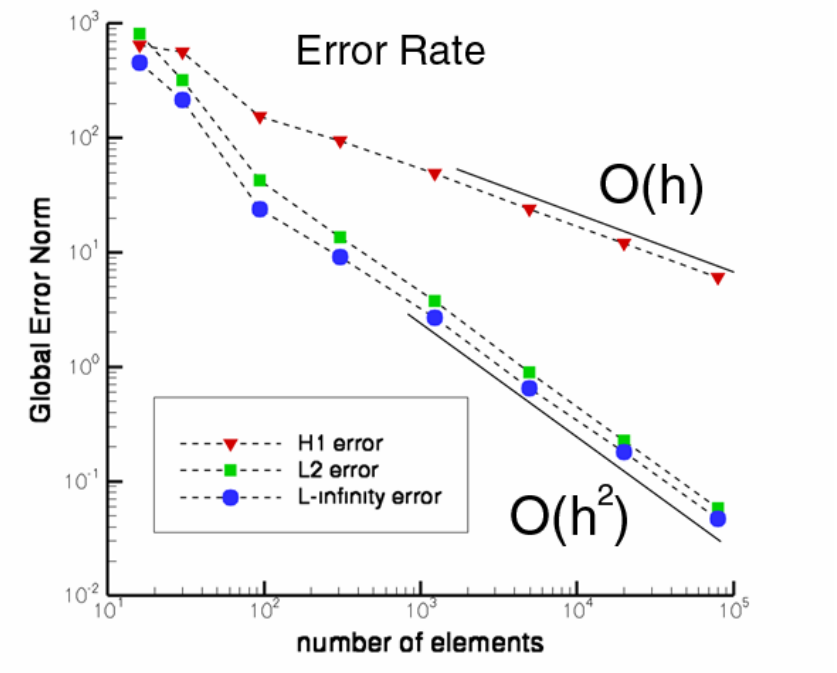

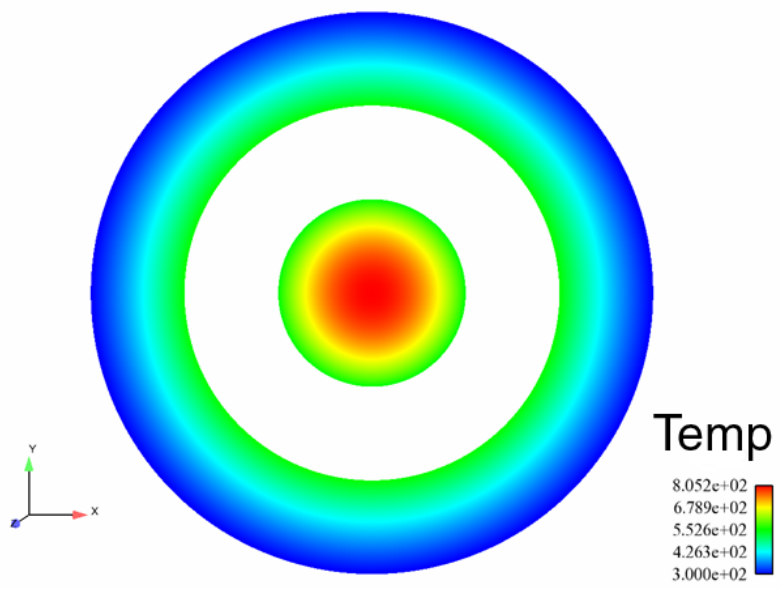

Verification of Mechanical Response

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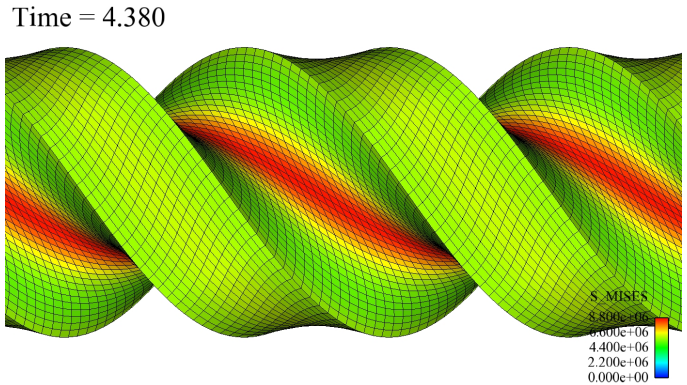
- This will involve Encore tools for norms, transfers, manufactured solutions, and error estimators.



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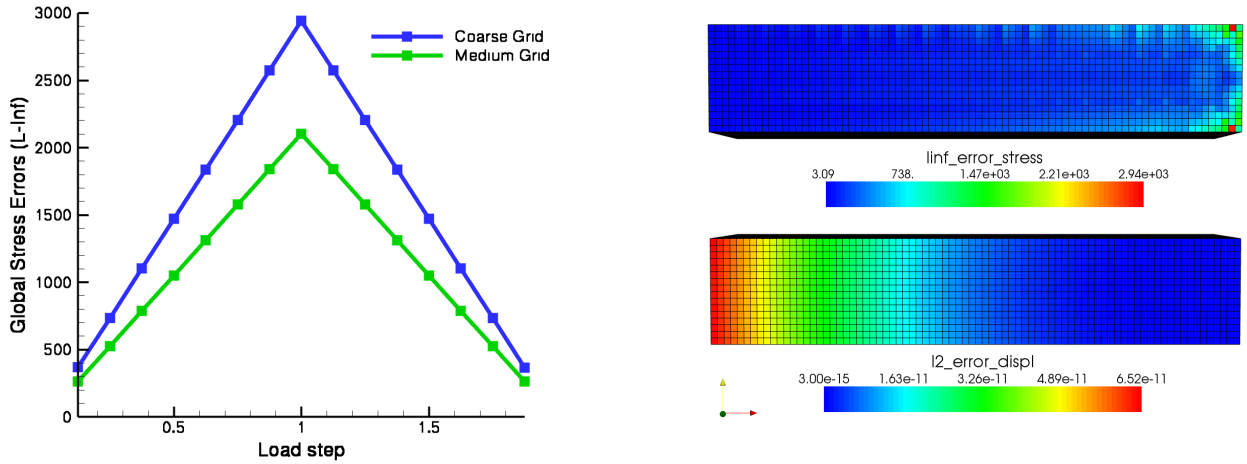

Figure: (left) Stress error rates (right) Stress/displacement error distribution

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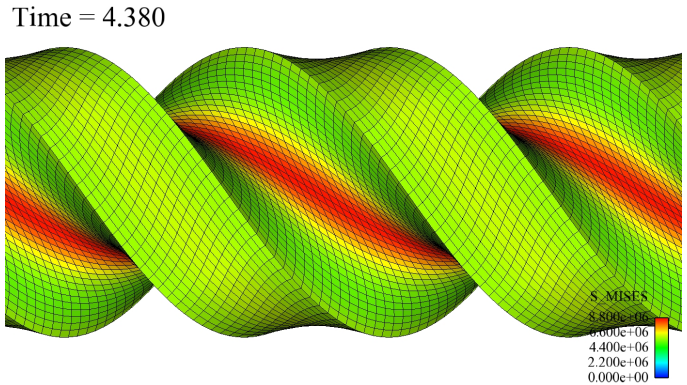

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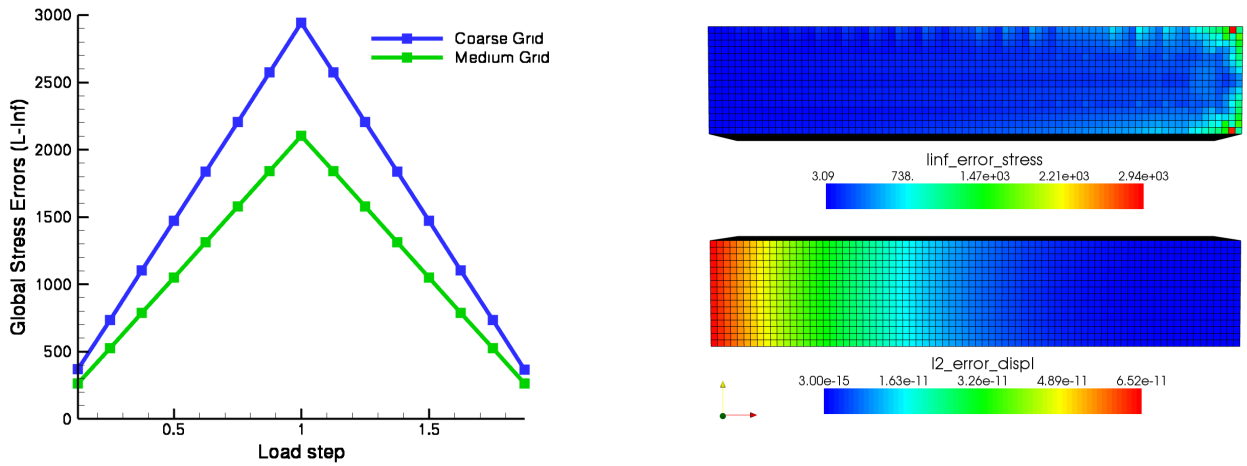

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Integral Based PPs

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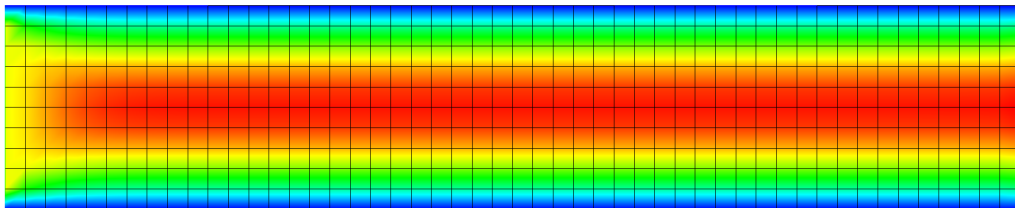
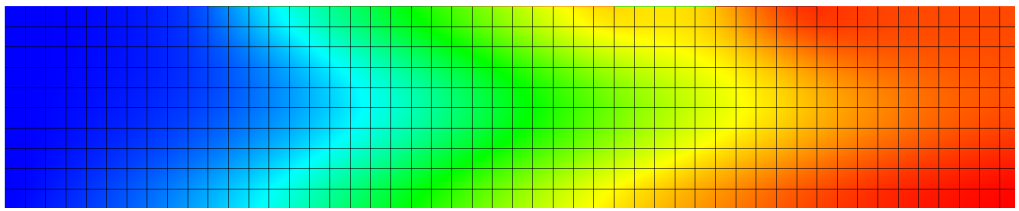


X Velocity Component.



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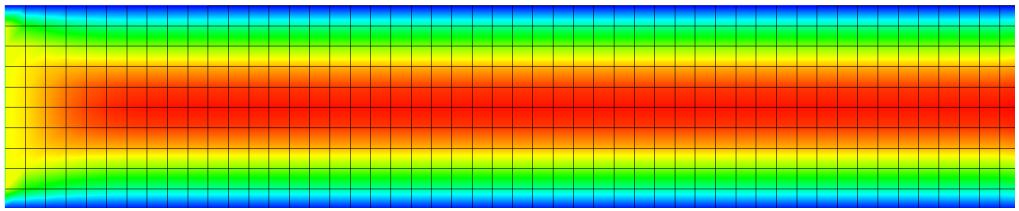

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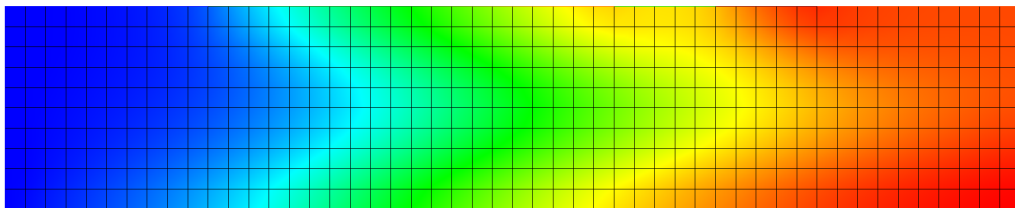

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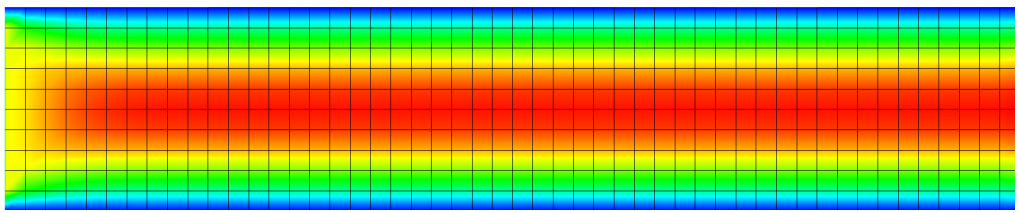

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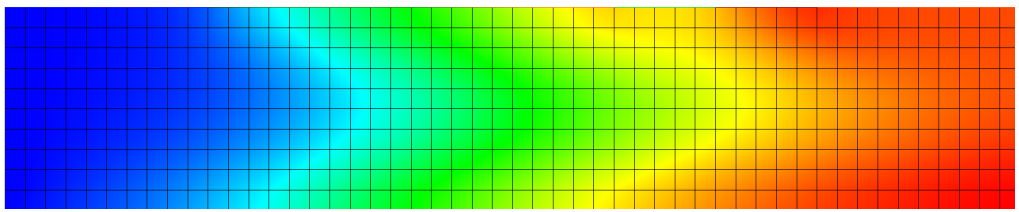

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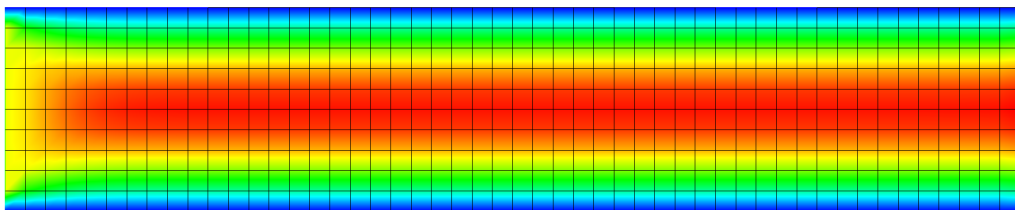

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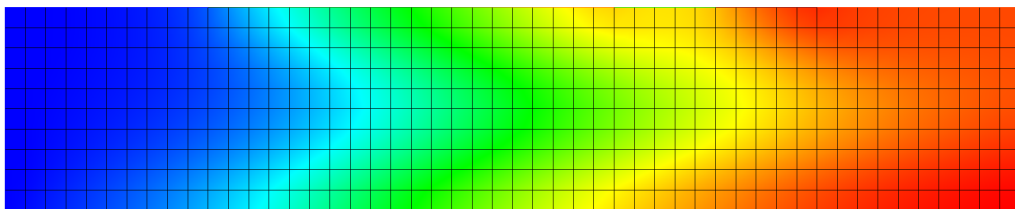

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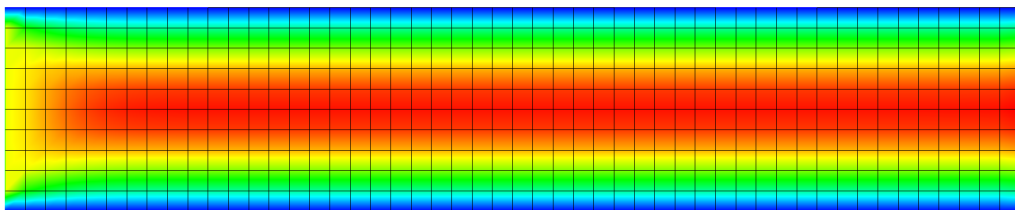

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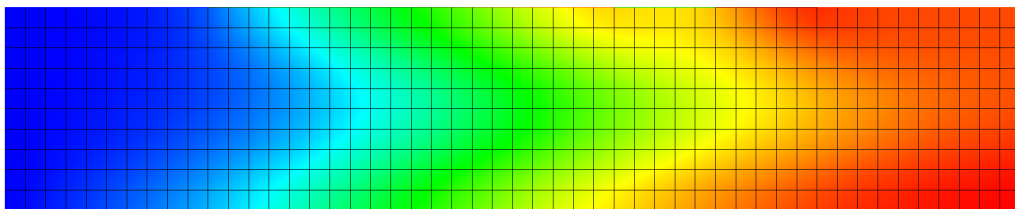

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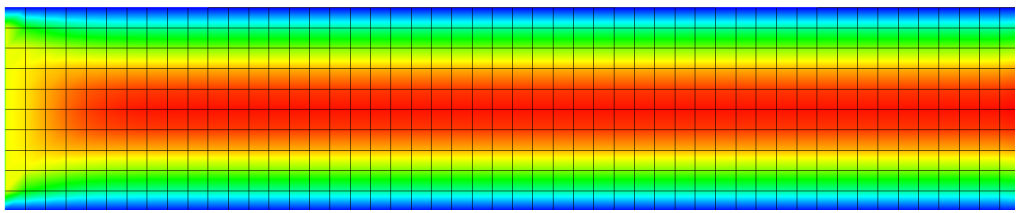

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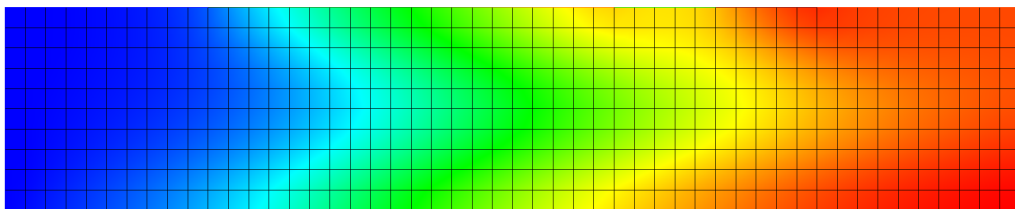

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Postprocessors That Create Fields

- Often users need to calculate auxiliary simulation fields for analysis or to feedback into the simulation.
- **Import Field** reads a field from an Exodus file.
- **Create Field** allows for creation of any size and type of field.
- **Interpolate Function** takes a Function, interpolating it into a nodal or element field.
  - Allows visualization of an analytic Function.
  - Useful for viewing the difference between two Functions.
  - If the values of a Function are derived from a material property, then you can visualize an interpolation of that property into an element field.
- **Recover Function** performs nodal patch recovery on a field. Useful for higher order recovery or nodal recovery of an element field (such as stress).

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- In online mode, **Encore** can access material properties for calculating heat flux.
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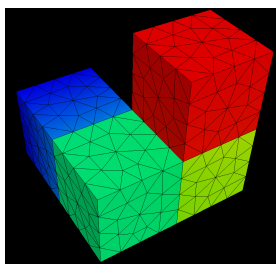
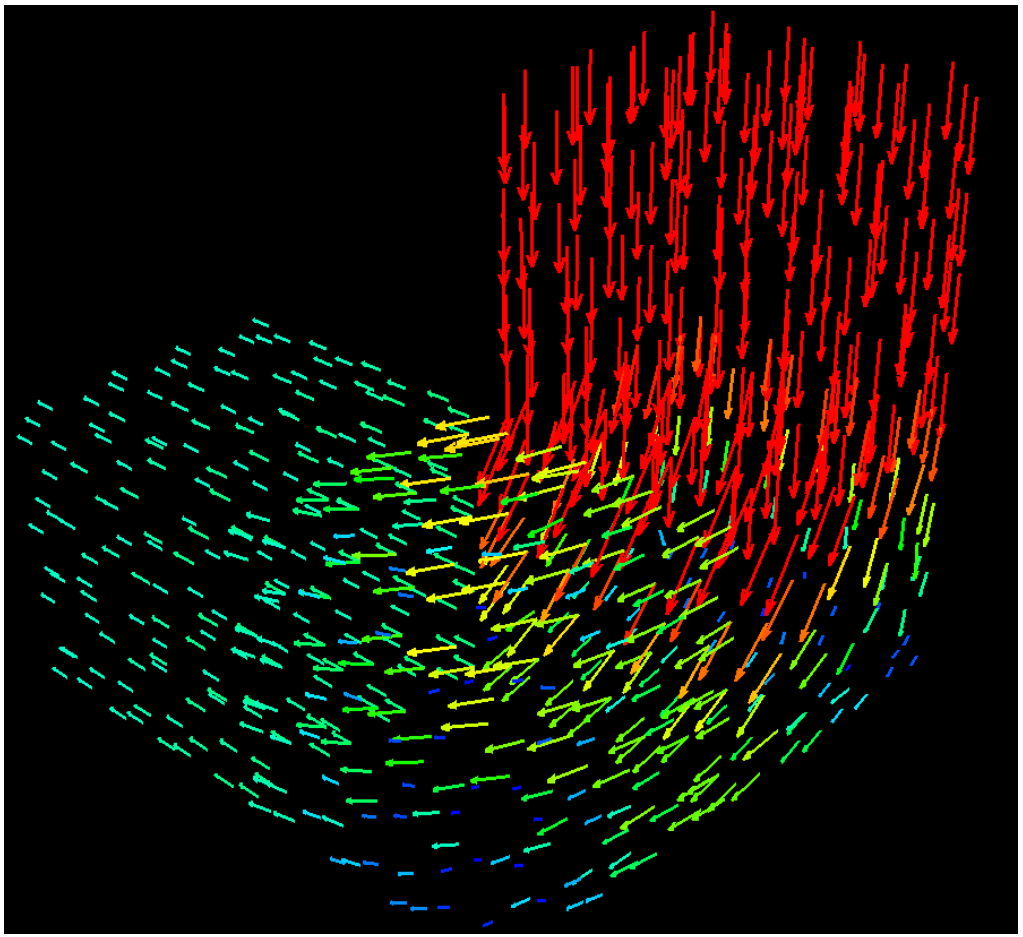
- Example: transient **Calore** simulation with thermal contact between blocks.





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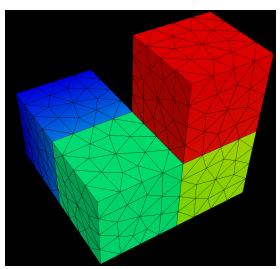

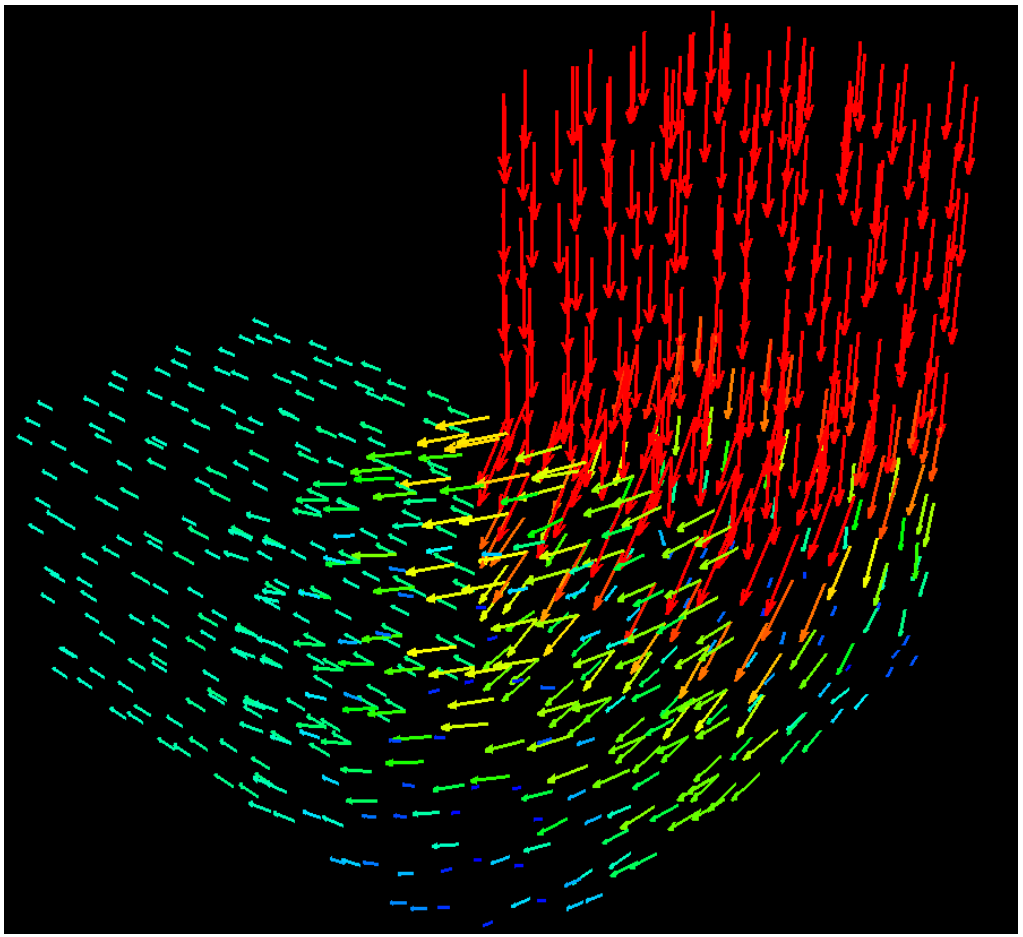

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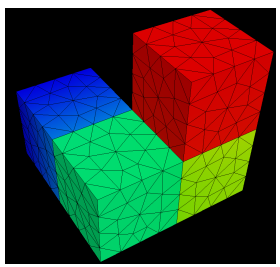

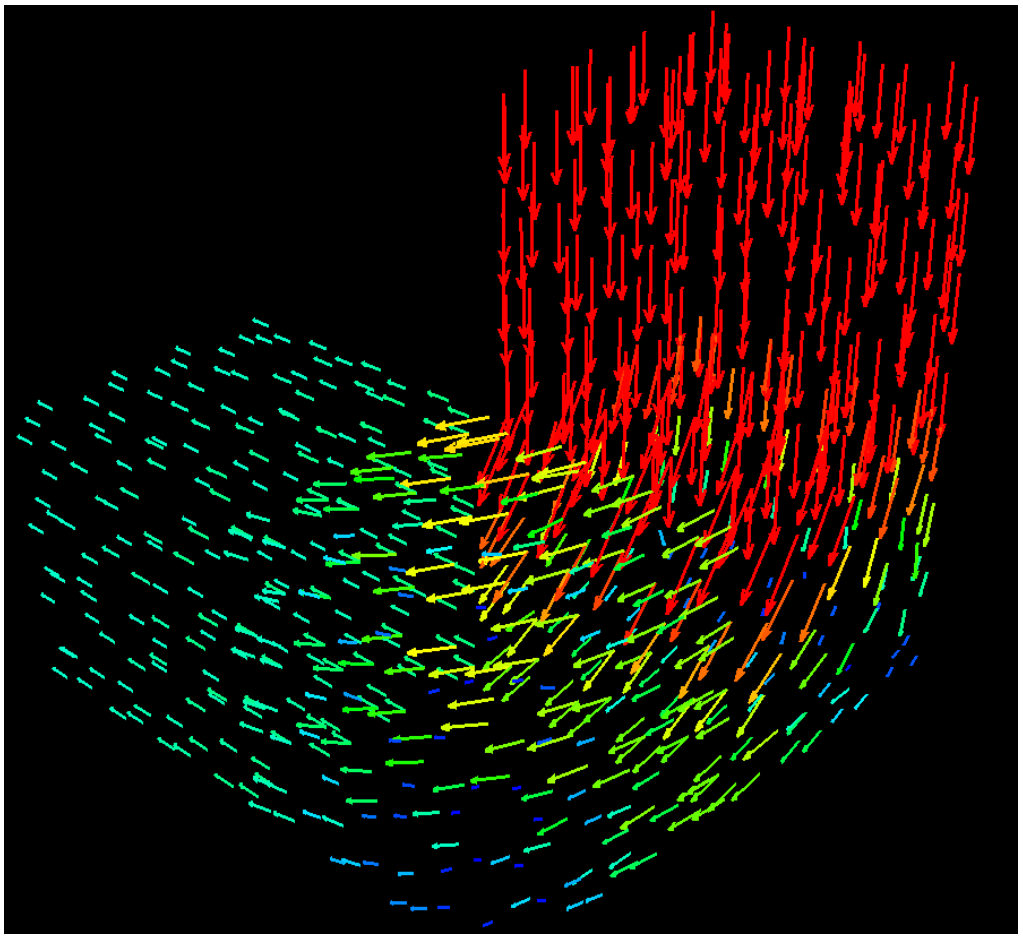

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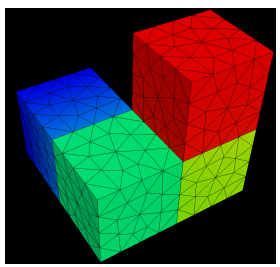

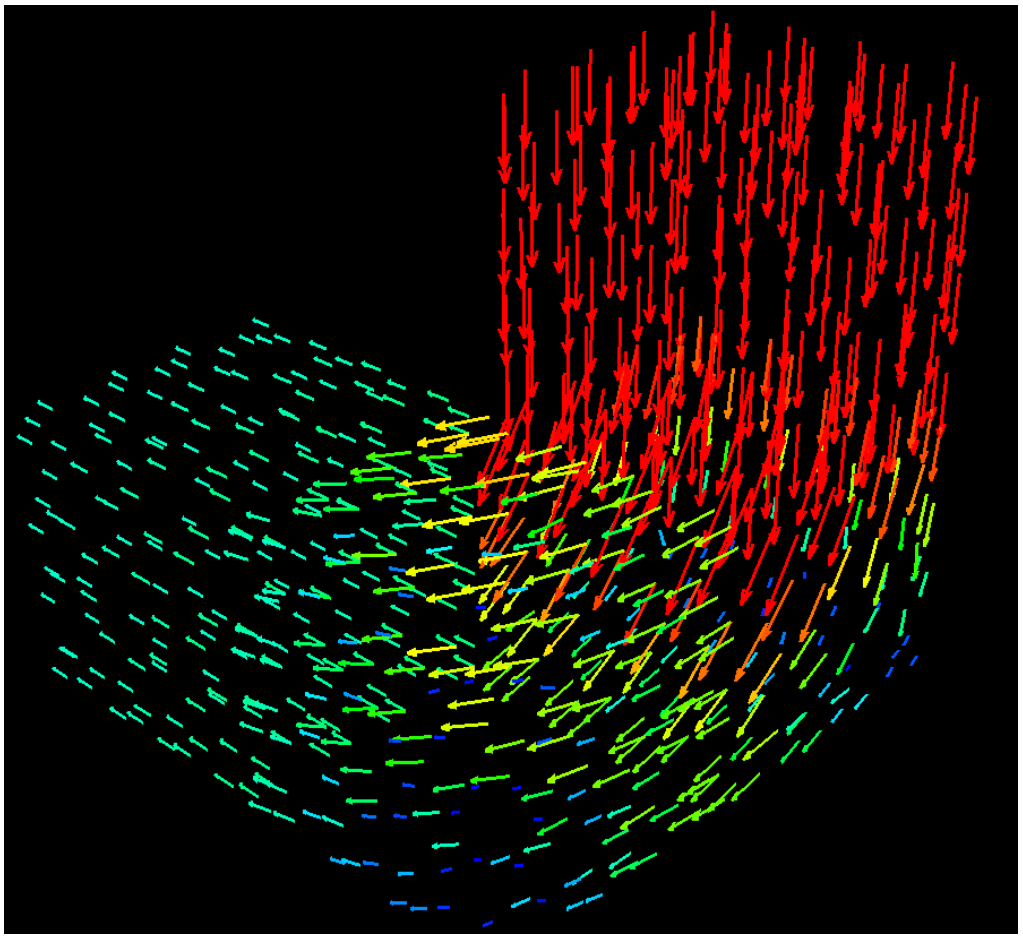

Example: Recover Function PP

- Stress recovery (averaging) is a common technique in solid mechanics.
- This can be used for postprocessing or to create an error estimator.
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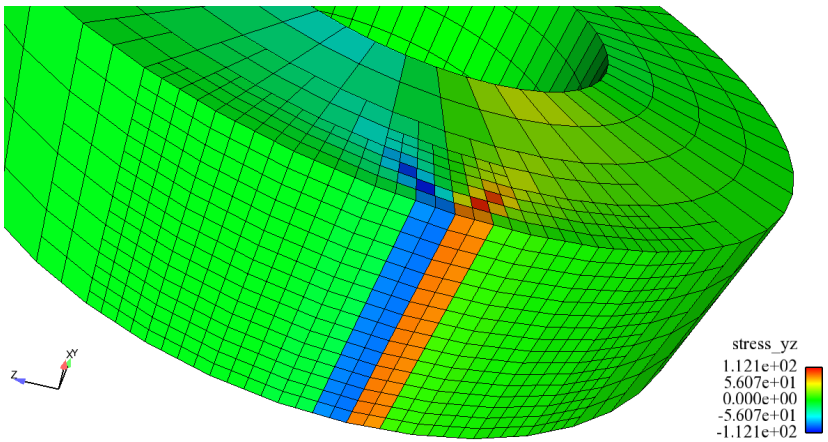
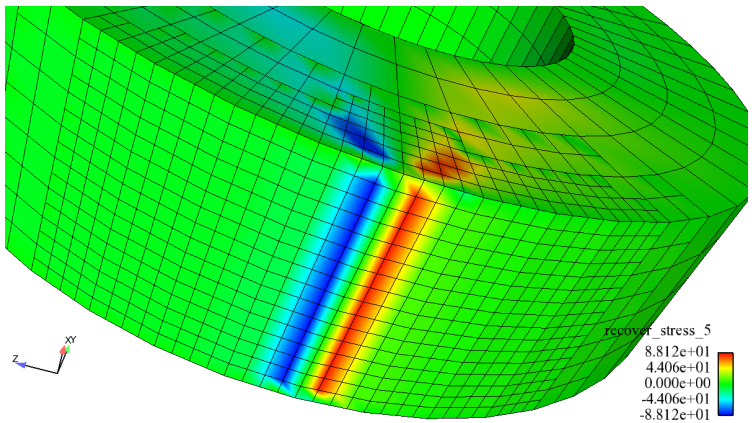


Element σ_{yz}



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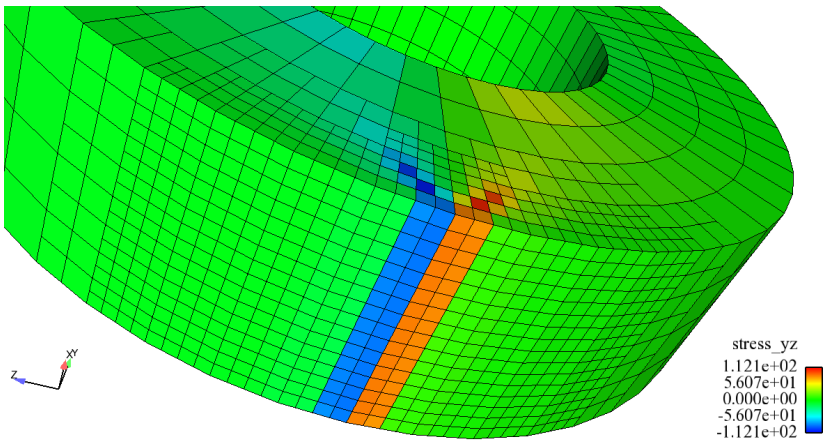

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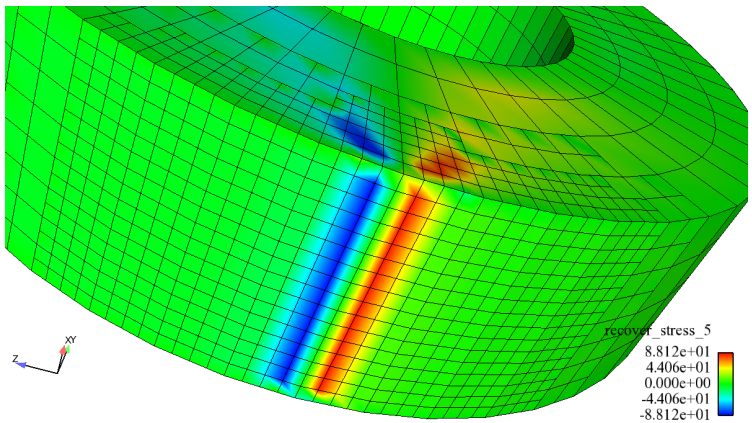

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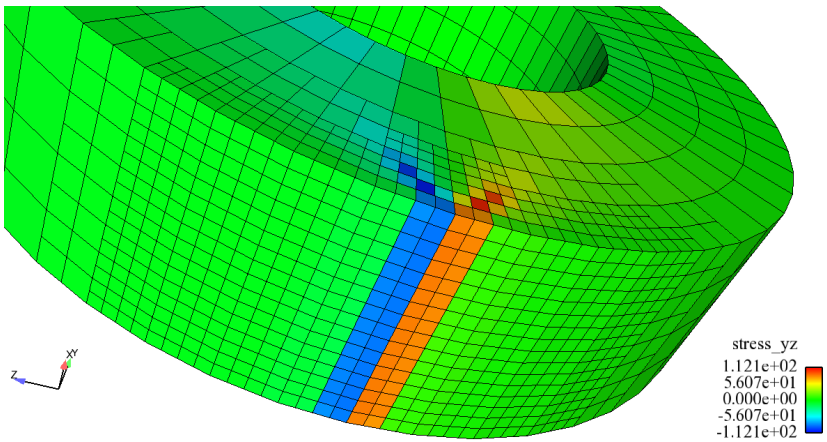

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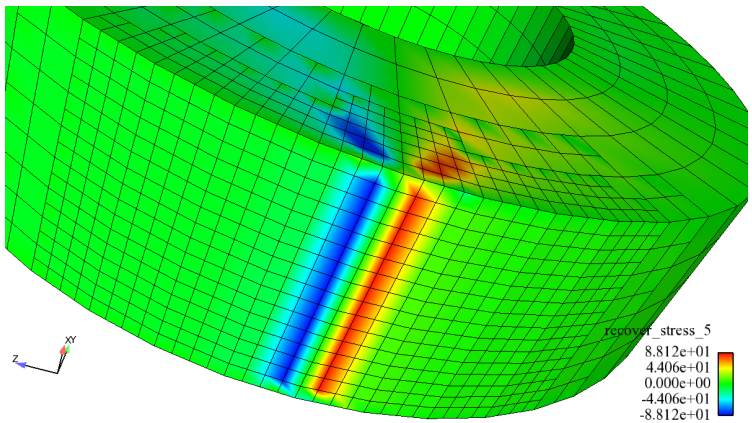

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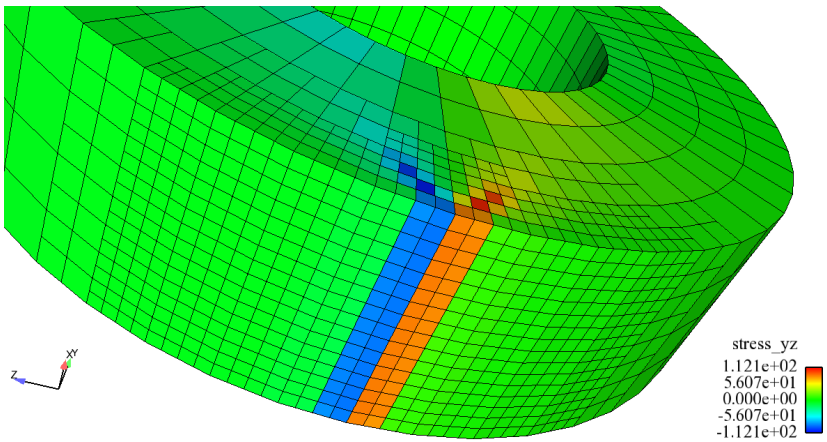

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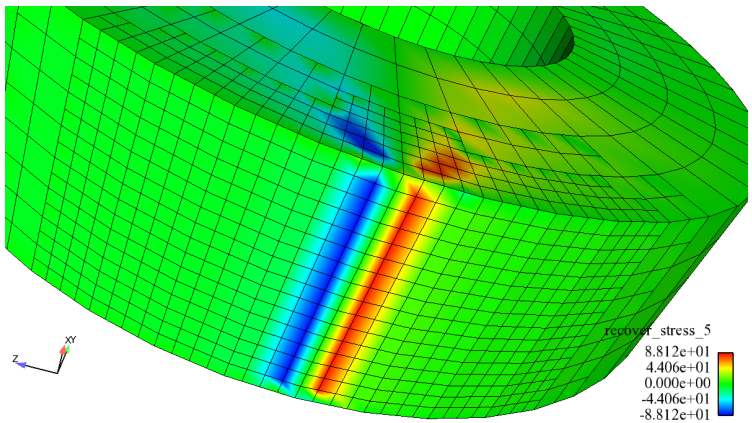

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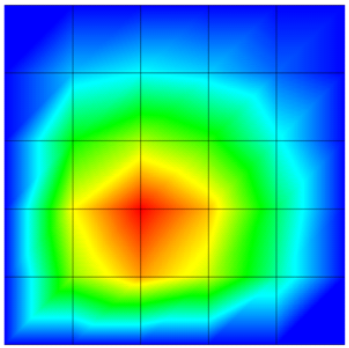
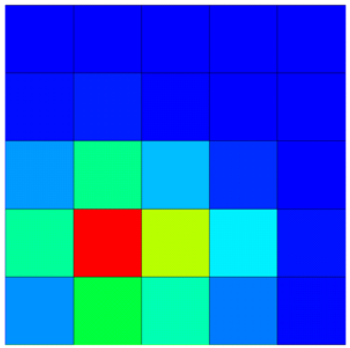
Transfers

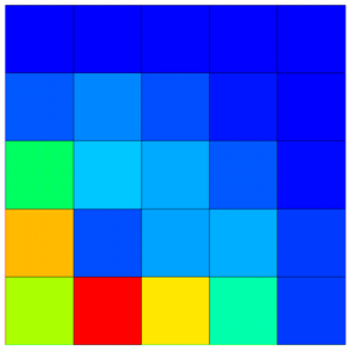
- Transfers project solutions from one mesh to another.
- This allows for solution comparison on different grids.
- 3 types of transfers: Nodal, Element, Quadrature.



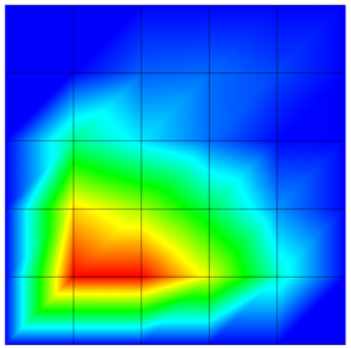
Coarse grid solution



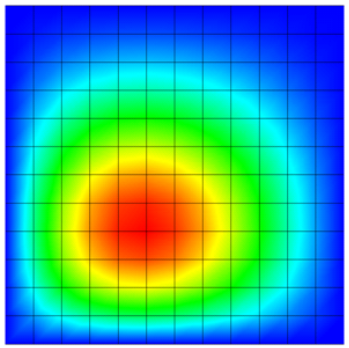
L2 error



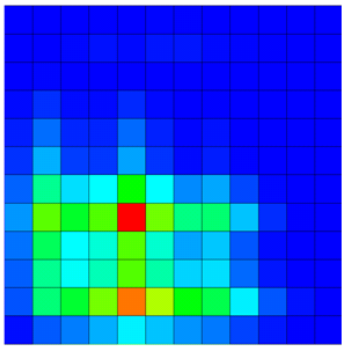
H1 error



Nodal error



Fine grid solution



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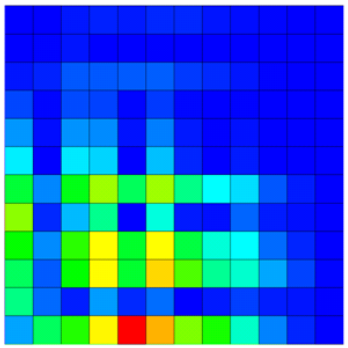

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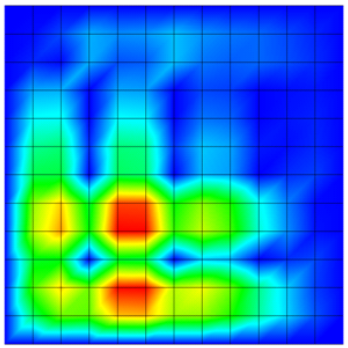

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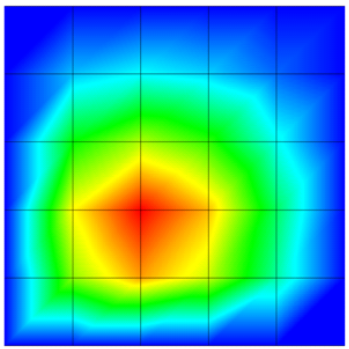
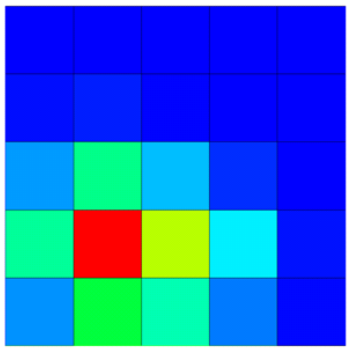
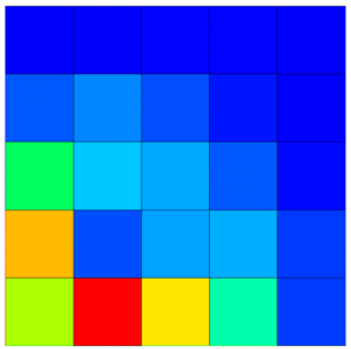


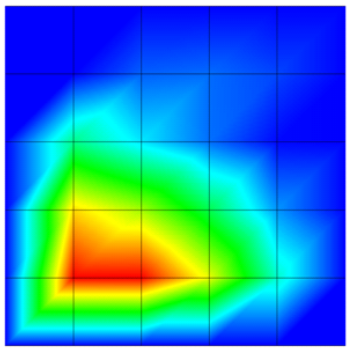
Coarse grid solution



L2 error



H1 error



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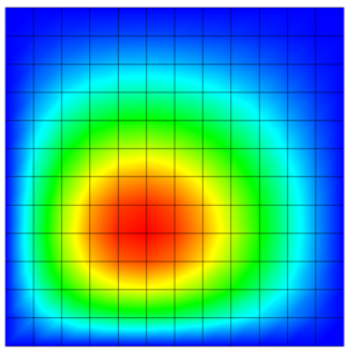
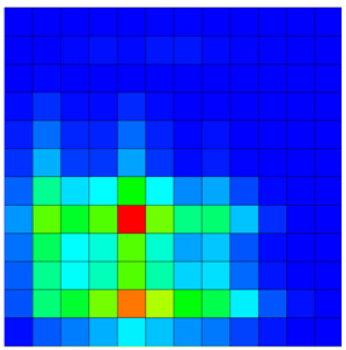
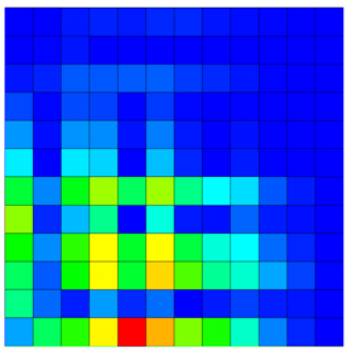


Fine grid solution



L2 error



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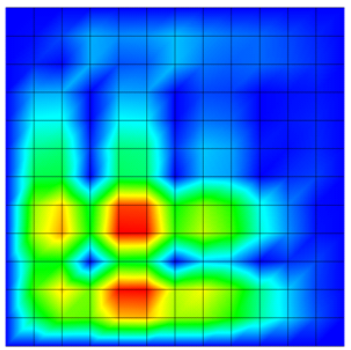

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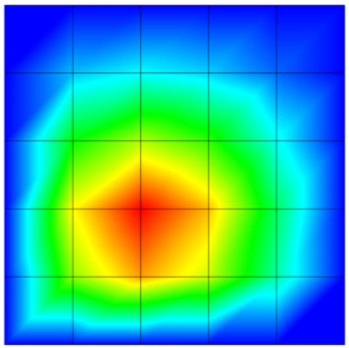

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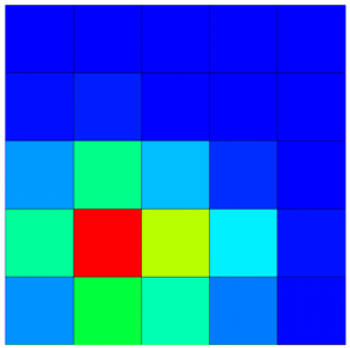

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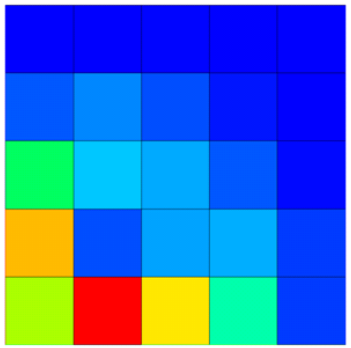

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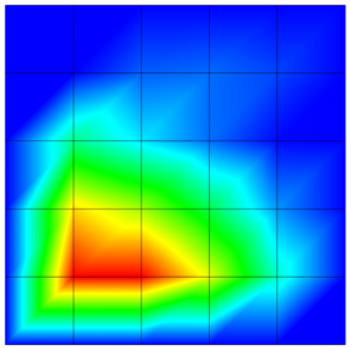

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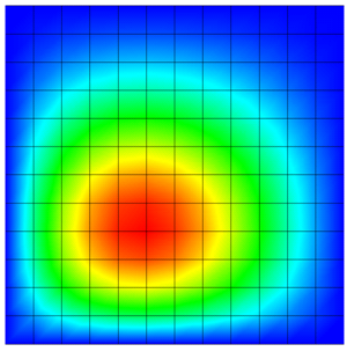

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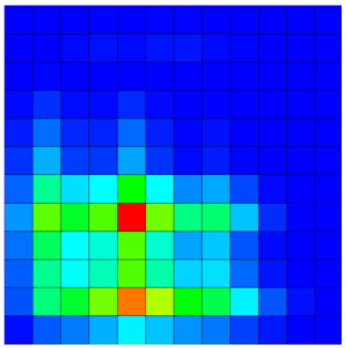

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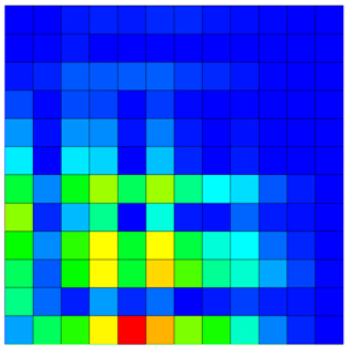

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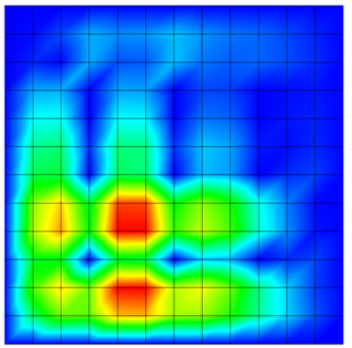

Nodal error

Impact: Transfers for Simulation Comparison

- A **Calore** customer noticed a discrepancy between runs done in **Coyote** and **Calore**.
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- Being able to visualize the differences led to finding a bug in the way triangles were being handled in the Calore input file.

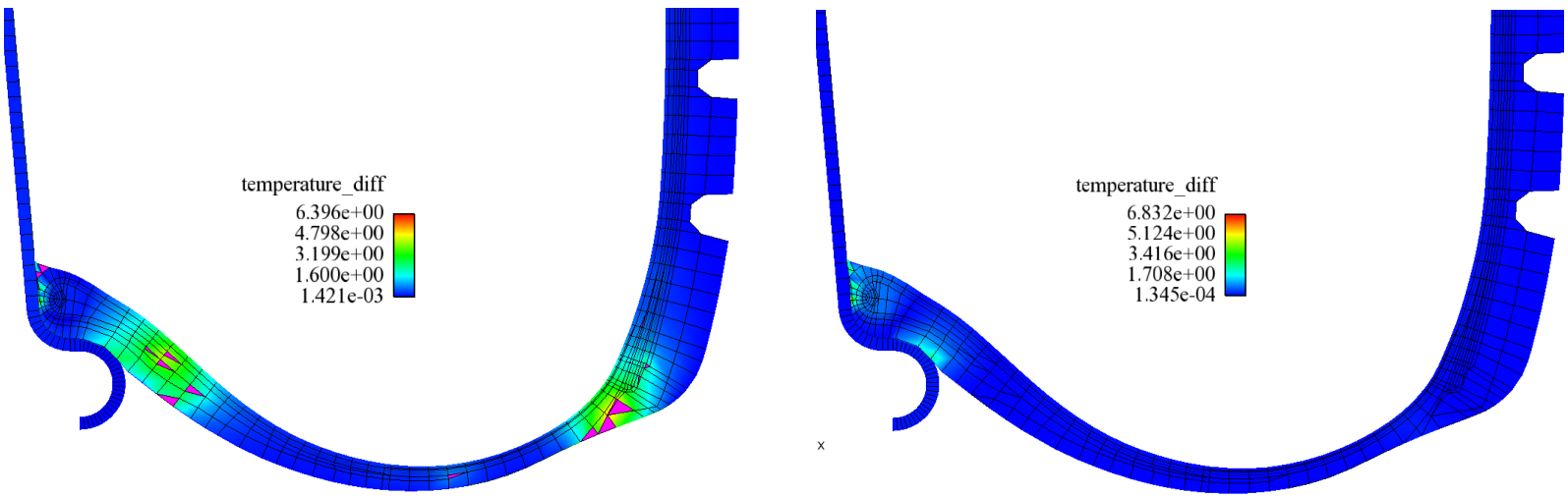

Figure: Temperature difference before and after bug fix.

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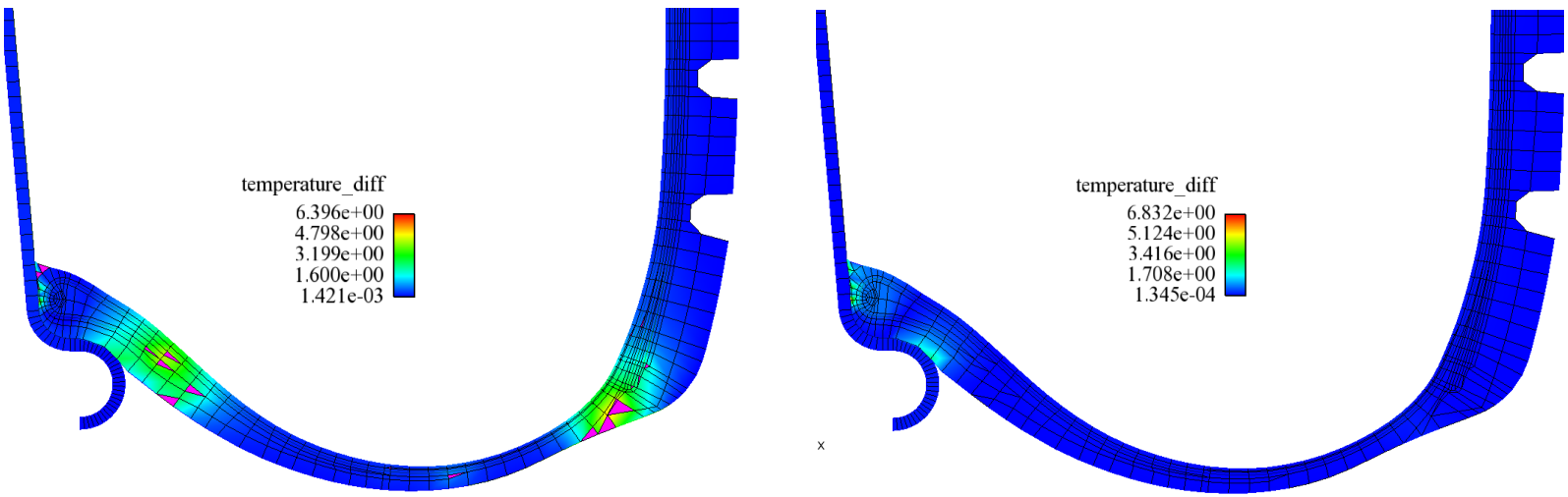

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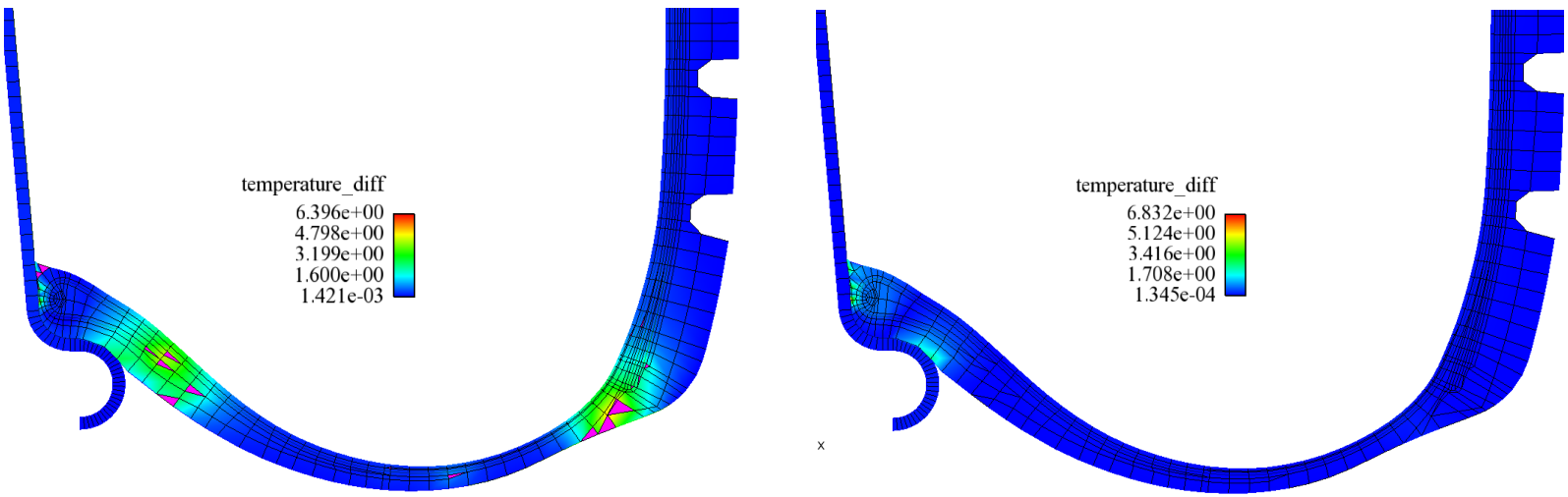

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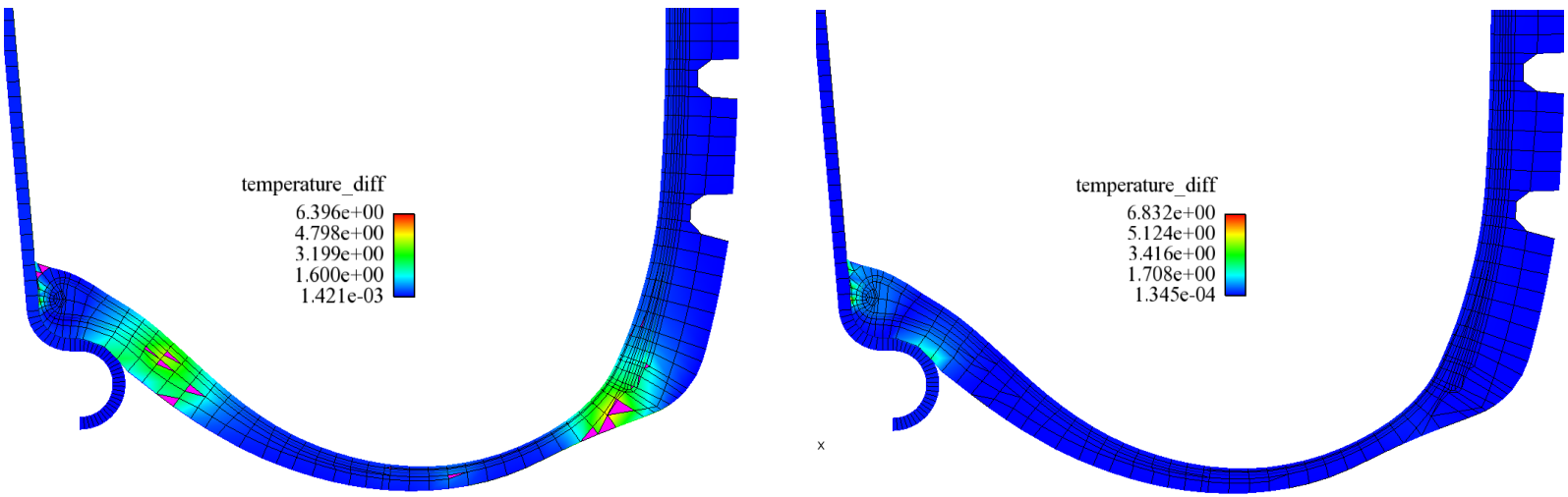
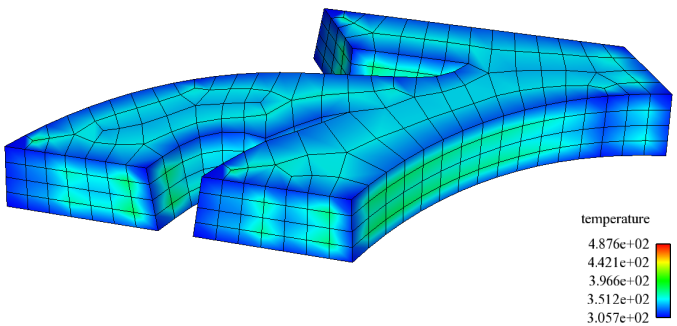


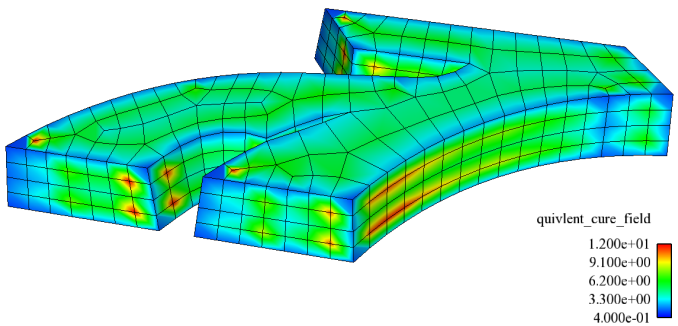
Figure: Temperature difference before and after bug fix.

Impact: User Postprocessor

- A User PP can be created allowing for complete flexibility to calculate whatever is desired.
- Writing a User PP is similar to a User Function.
- An external customer has used this capability to calculate a time integrated nodal quantity in both *online* and *offline* modes.



(a) Temperature.



(b) Time Integrated PP Value.

part 2

Error Estimation and Adaptivity

Overview of Error Estimation and Adaptivity

- The Adaptivity Cycle
- Physics Independent Error Indicators
- Adjoint Based Error Estimators
- Markers
- User-Driven Control of Adaptivity

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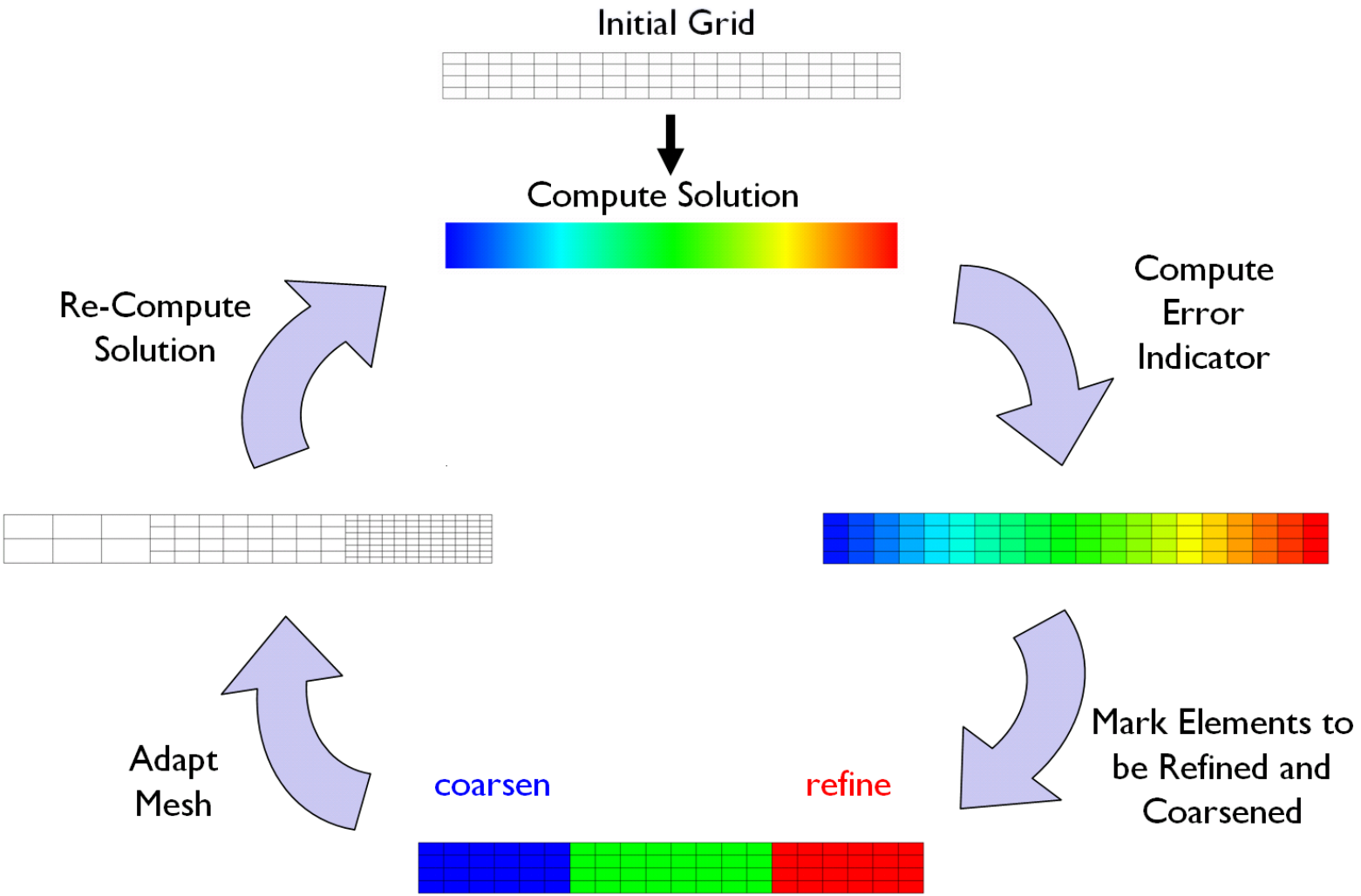
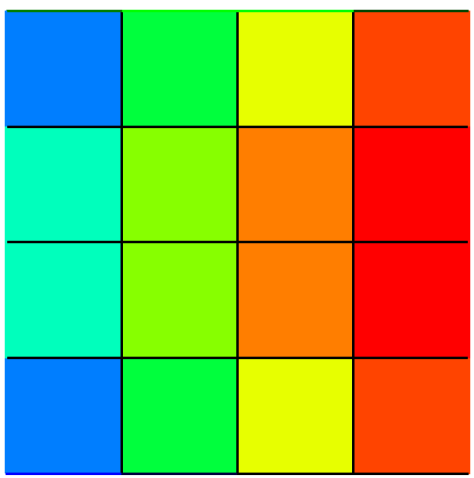
The Adaptivity Cycle

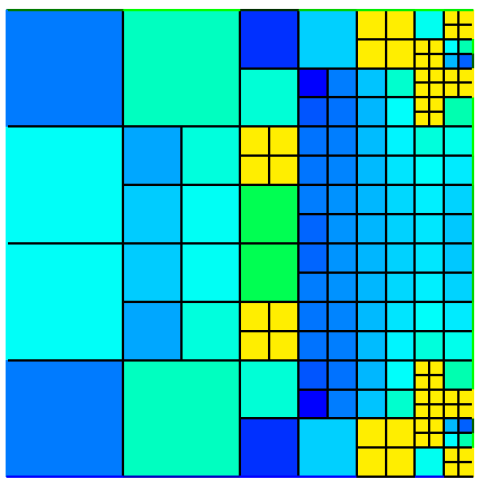


Physics Independent Error Indicators

- Error Indicators have two purposes:
  - Estimate the numerical error in the simulation on a given grid.
  - Provide input to mesh adaptivity, in the form of a spatial error distribution
- Encore implements several physics independent error indicators, allowing re-use in multiple application codes.
- Physics independent indicators operate solely on computed fields without knowledge of engineering/physics equations.



Error = 133%



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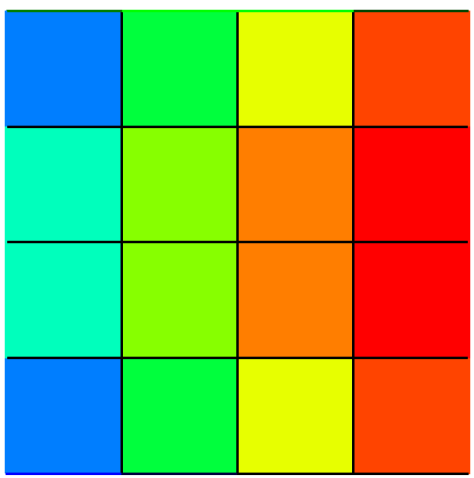

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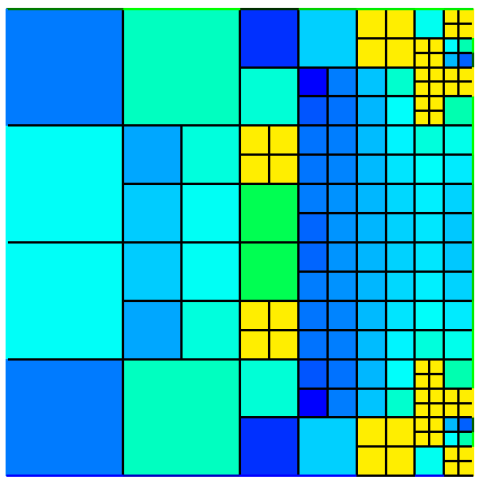

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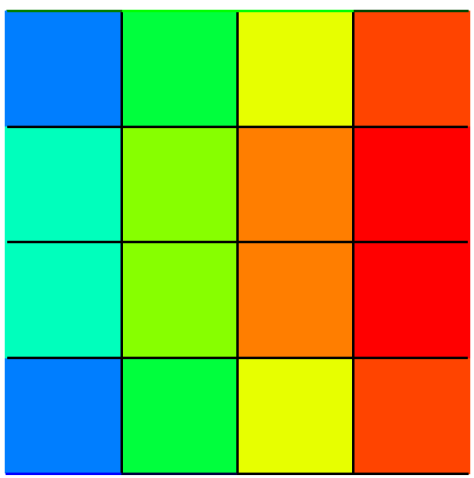

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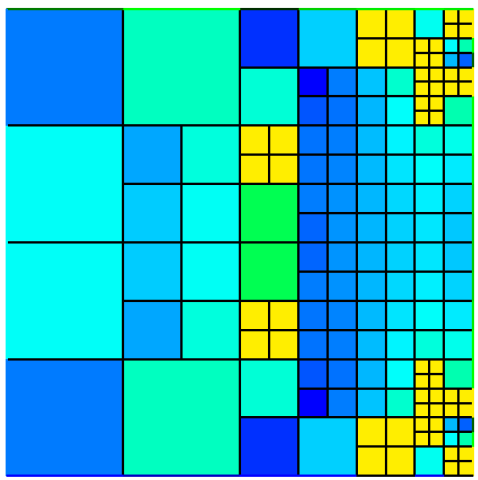

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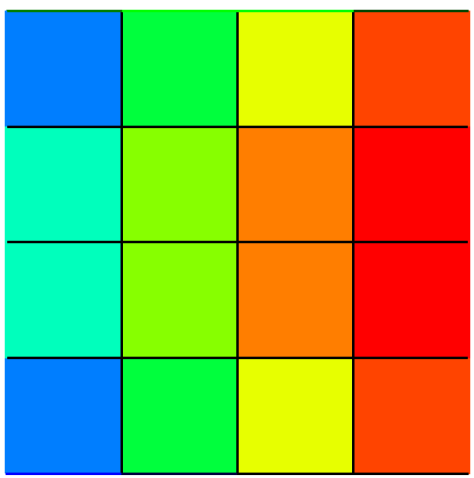

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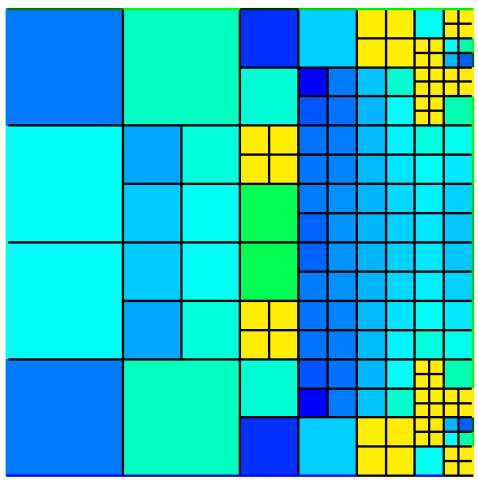

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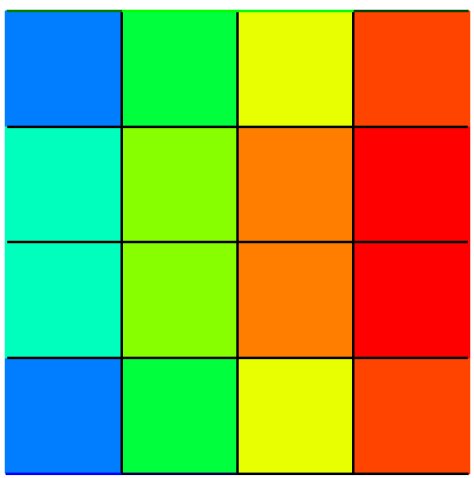

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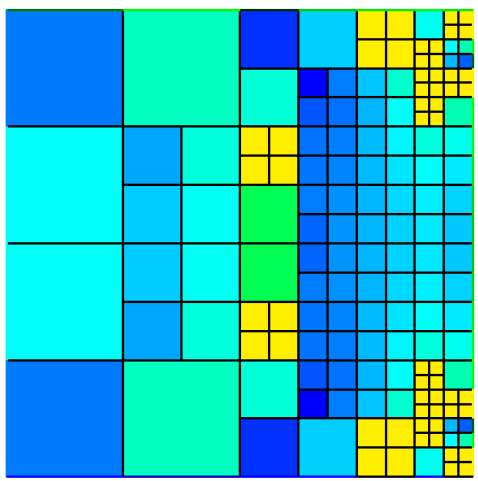

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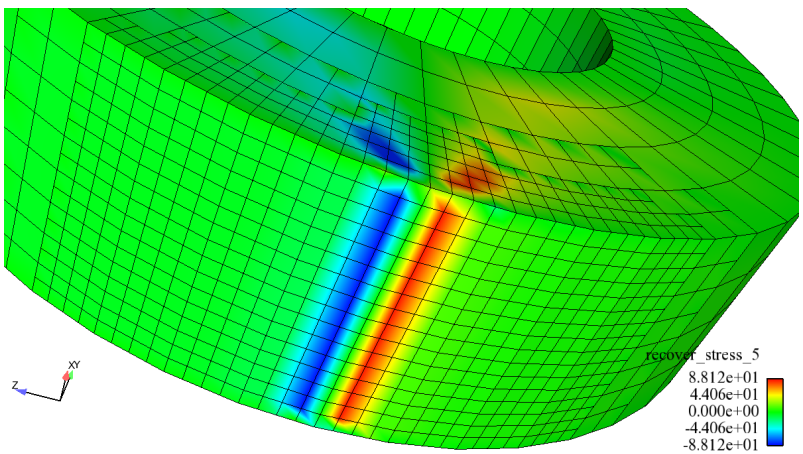
Recovery Indicator

- Recovery Indicator computes difference between flux/stress and recovered (averaged) flux/stress (ZZ estimator).

$$\|\sigma - \sigma_h\| \approx \|\sigma^*(\sigma_h) - \sigma_h\|$$

- Example: simplistic rolling tire result from **Adagio** using feature based refinement in a box.
- Figures are of tire surface that is in contact with the road.



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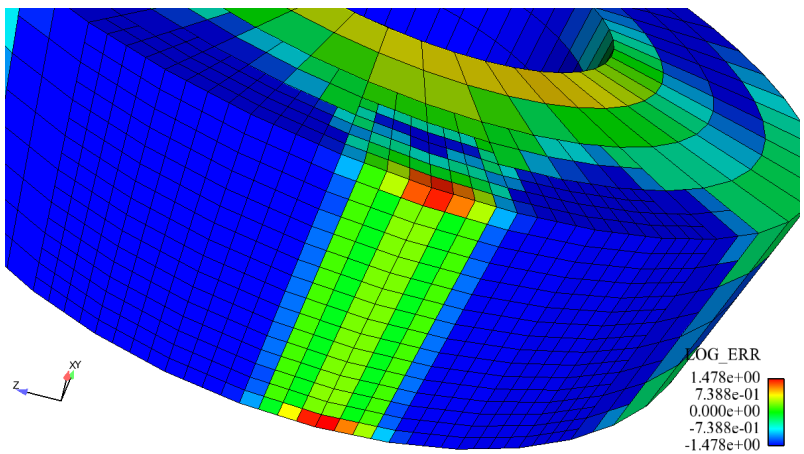

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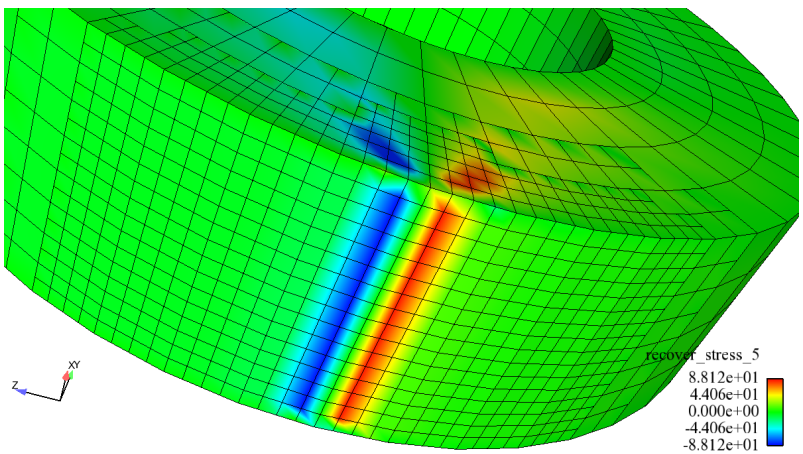

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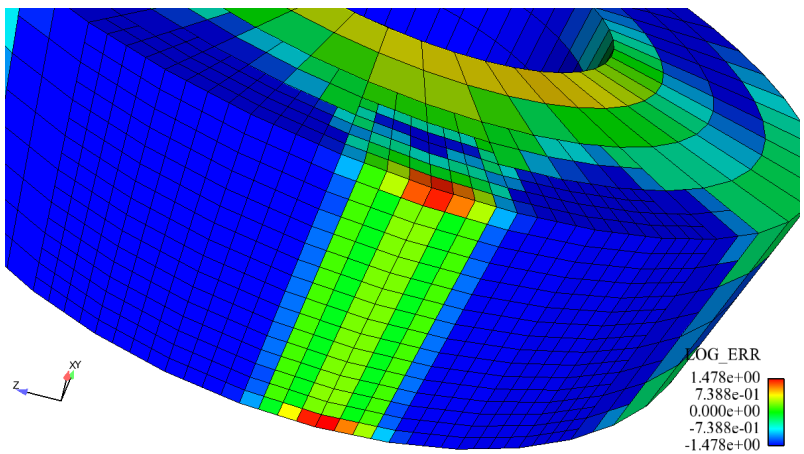

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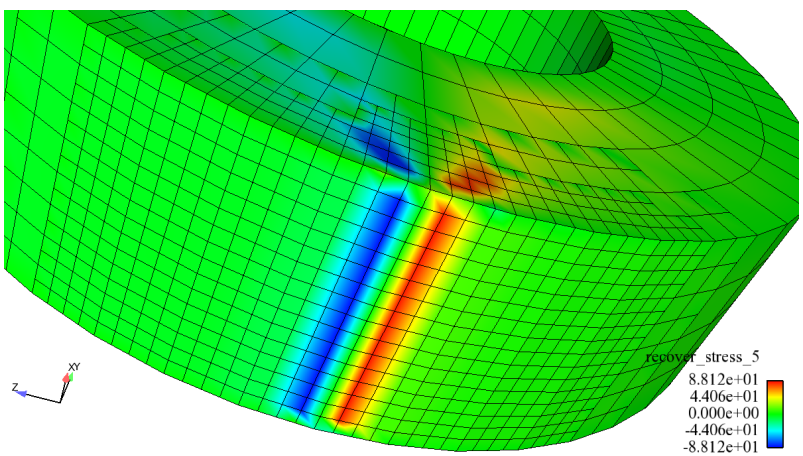

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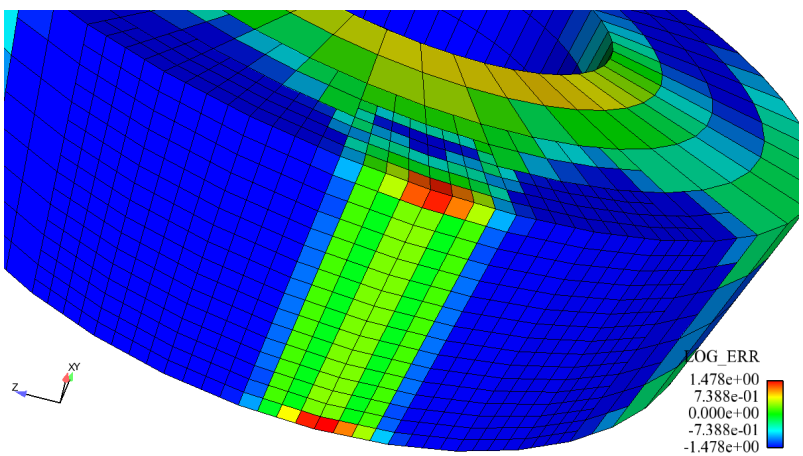

Log of Indicator

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- Jump Indicator computes jumps (residuals) across inter-element interfaces.
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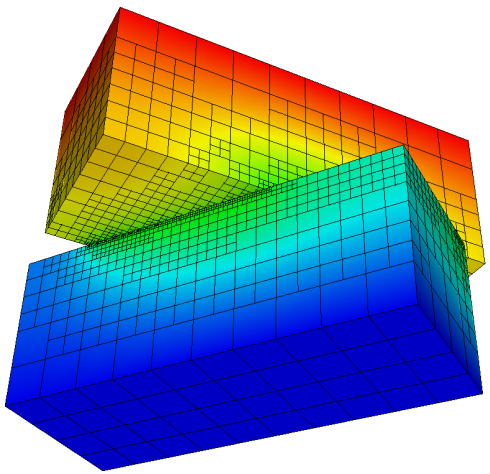
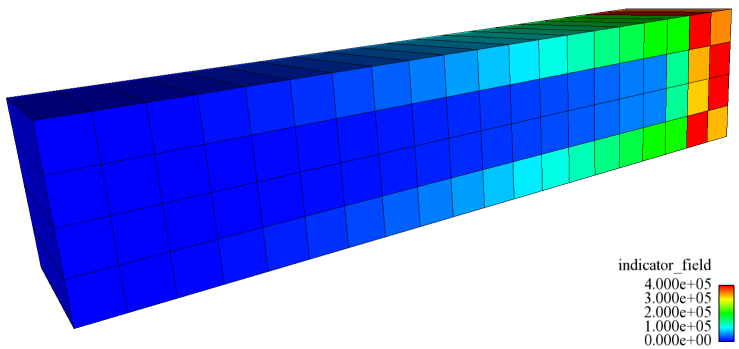


Calore thermal contact



Adagio stress jump

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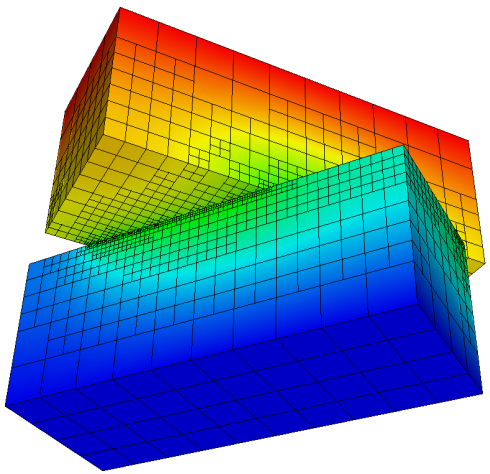

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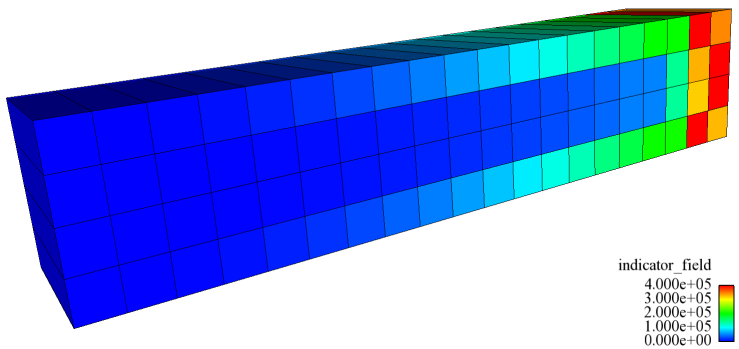

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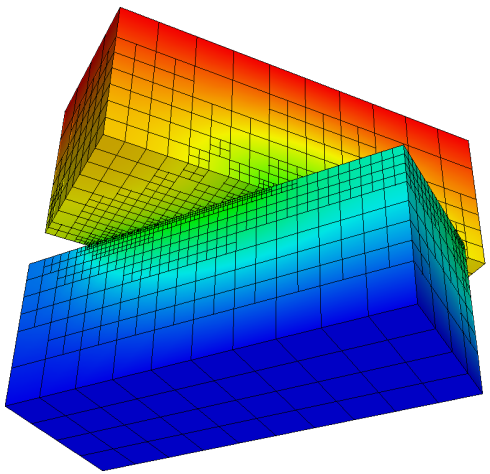

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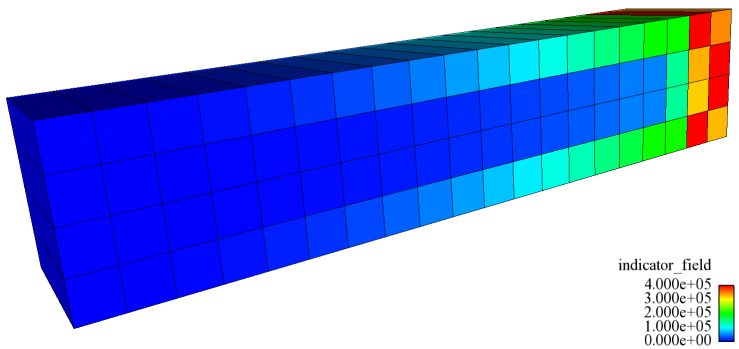

Adagio stress jump

Adjoint Based Error Estimators

- Often analysts are interested in specific outputs of a simulation, rather than simulation fields:
  - Point values
  - Integral/average values
  - Surface fluxes
- These outputs correspond exactly to Encore PPs.
- Adjoint based error estimators and adaptivity are targeted to produce accurate PPs with efficient use of resources.
- These error estimators require an auxiliary linear adjoint solve.
- An FY08 ASC funded project (Algorithm Integration) is working on this technology for Sierra Mechanics codes.
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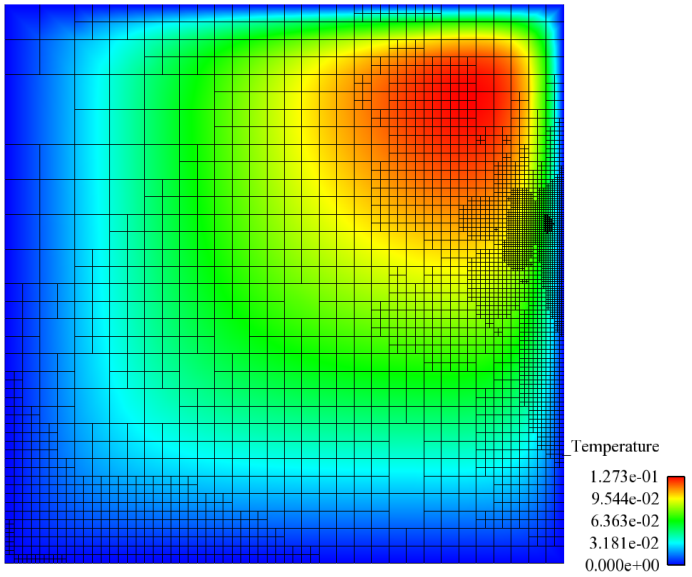

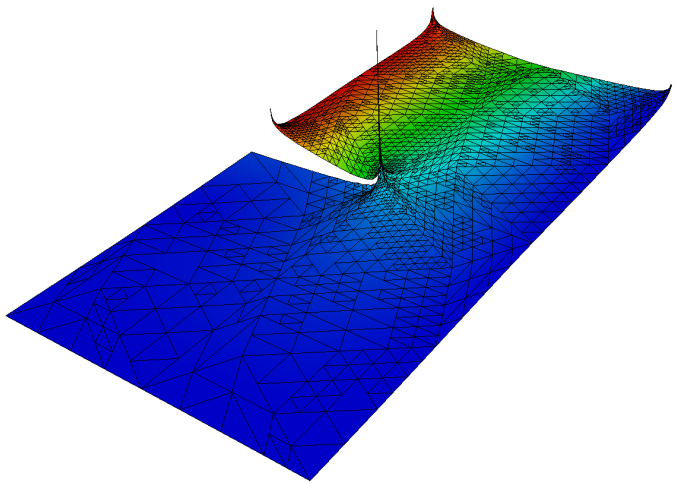

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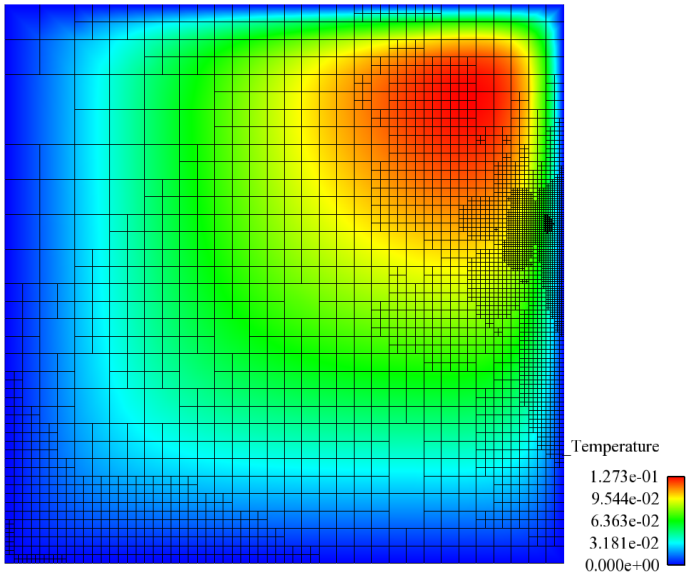

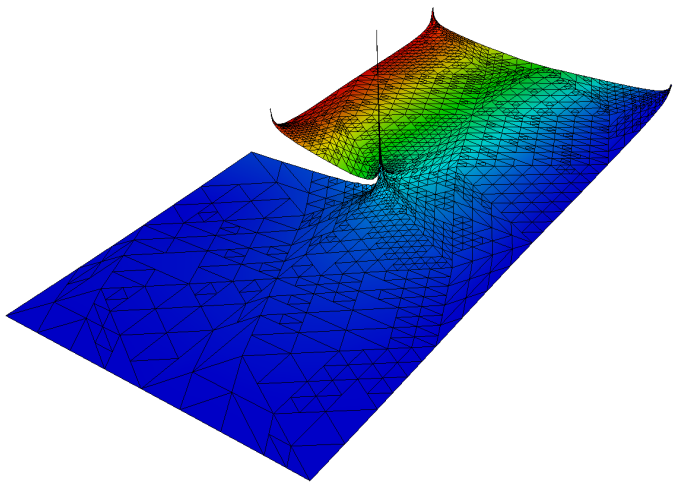

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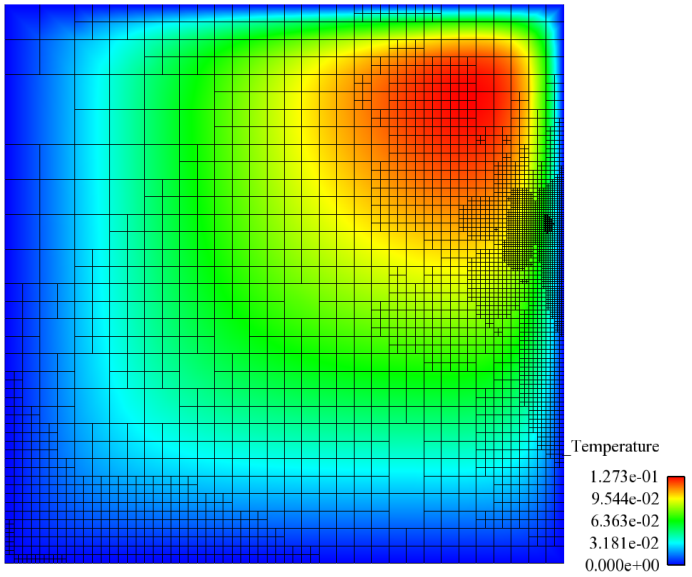

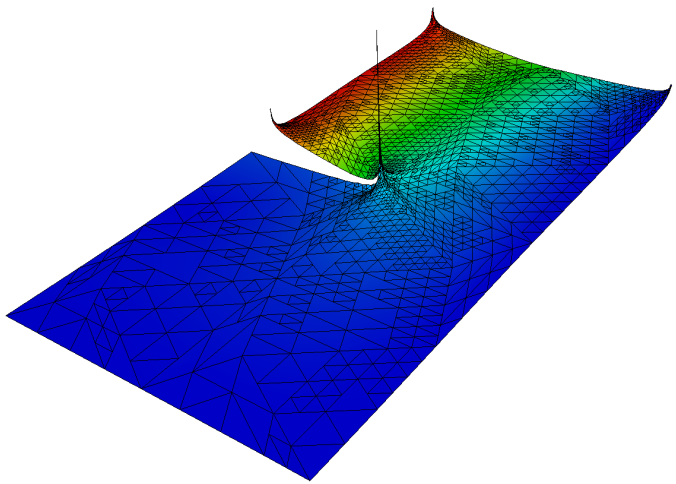

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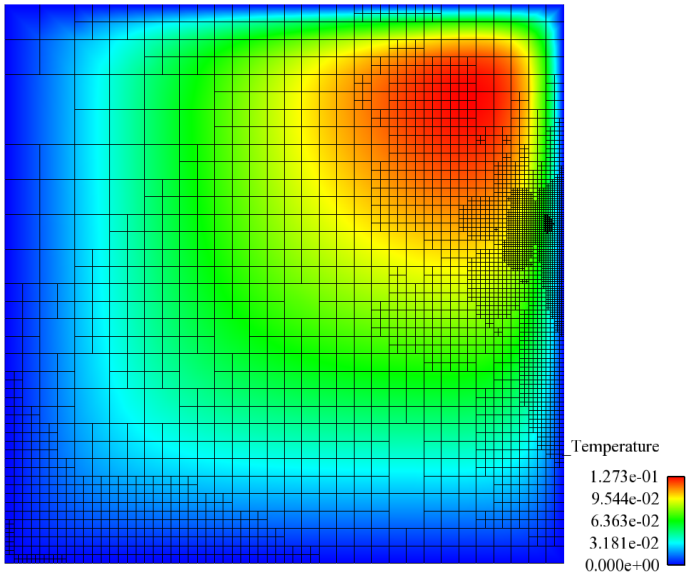

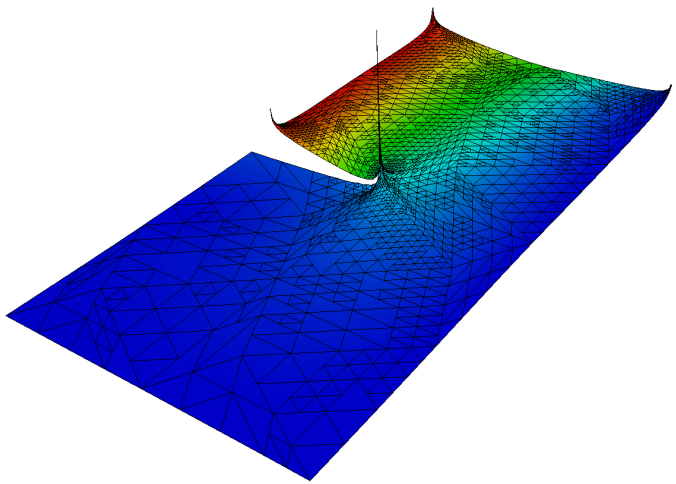

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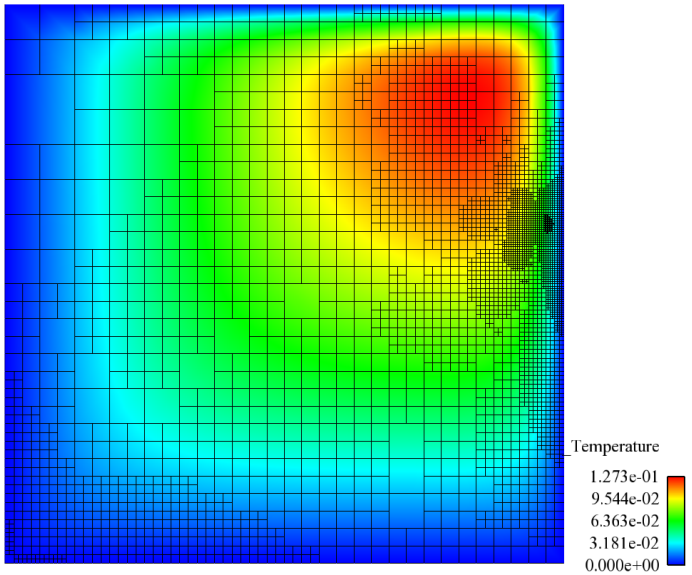

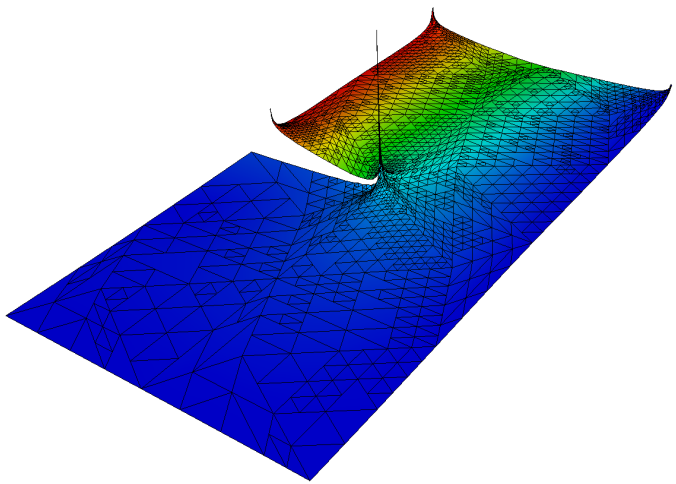

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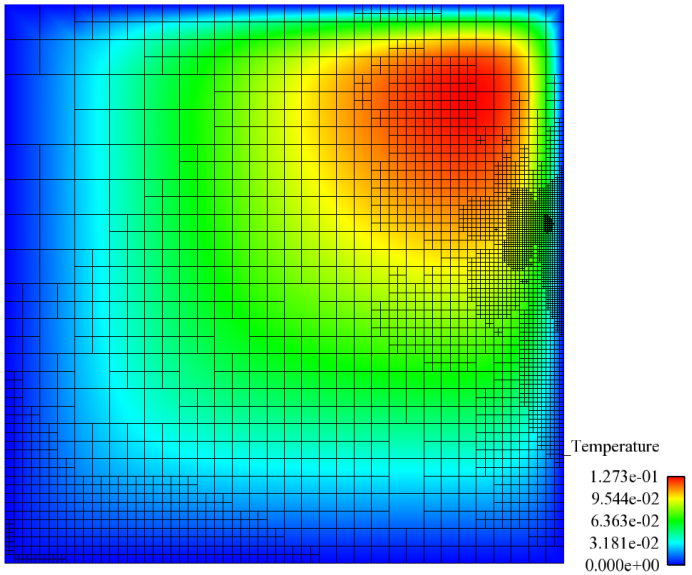

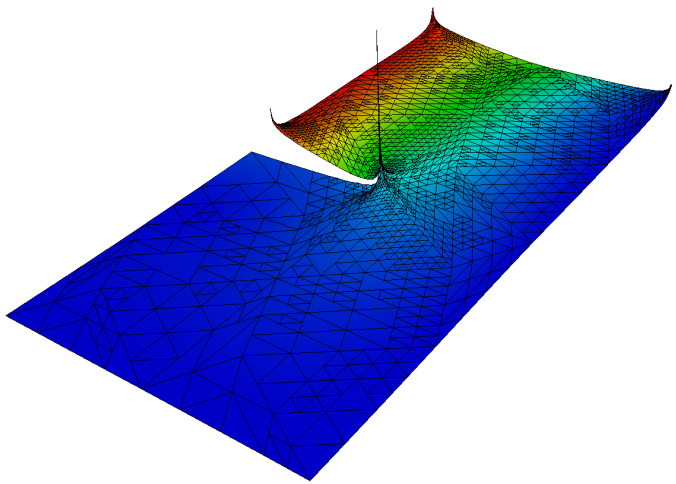

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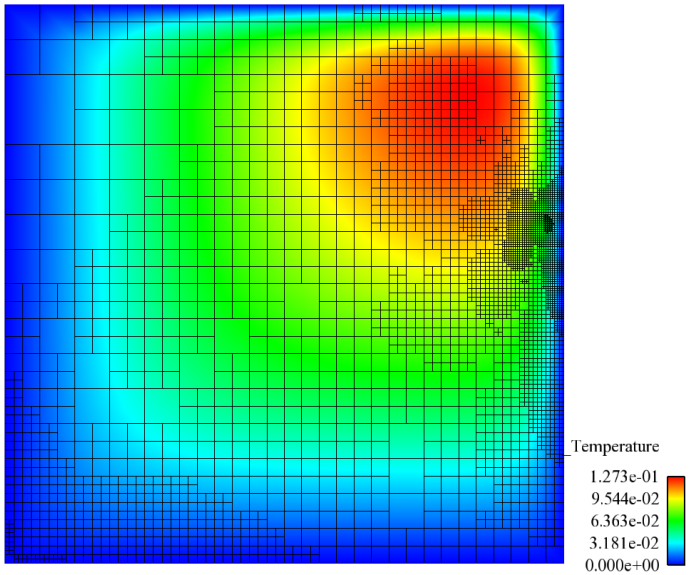

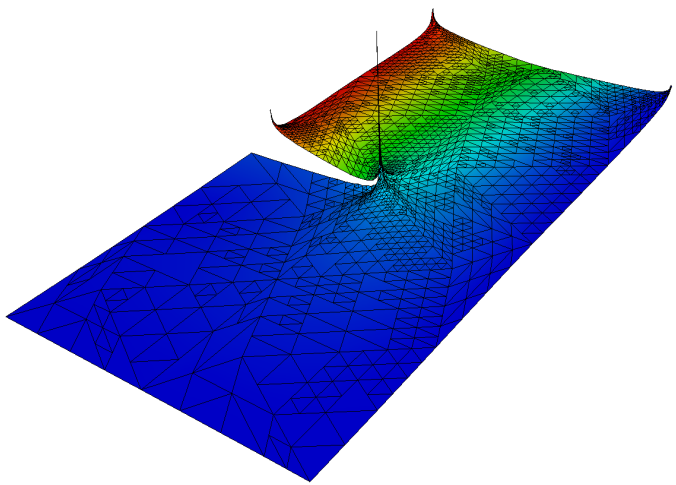

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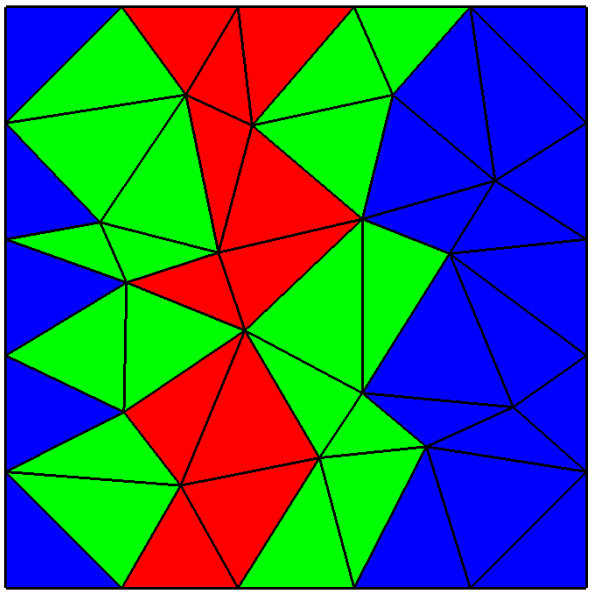

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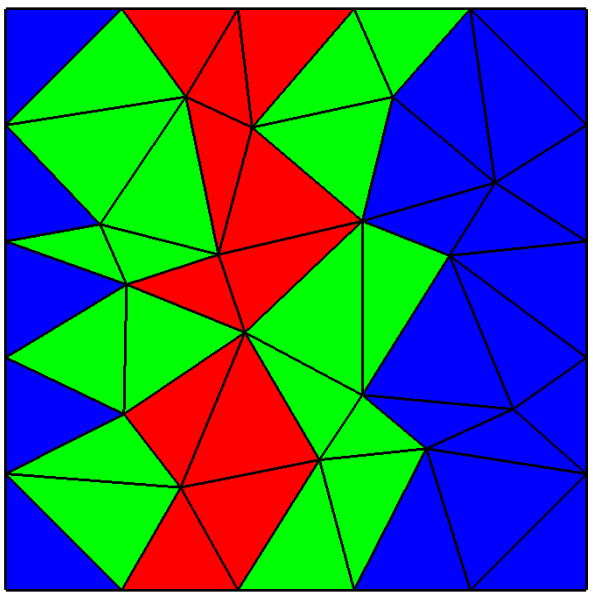

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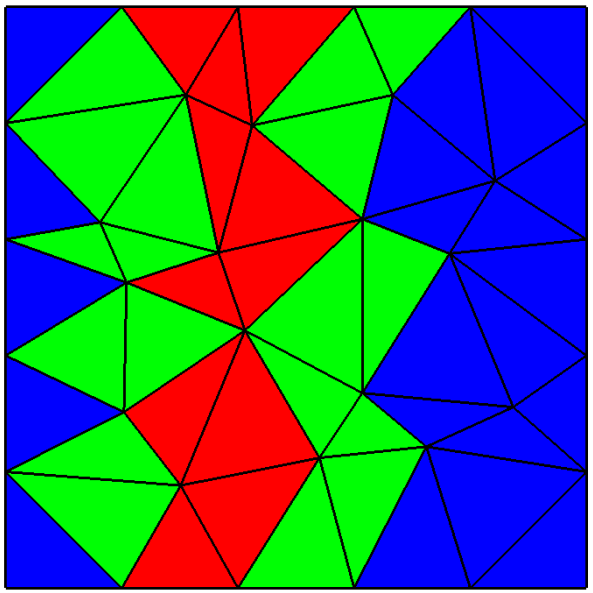

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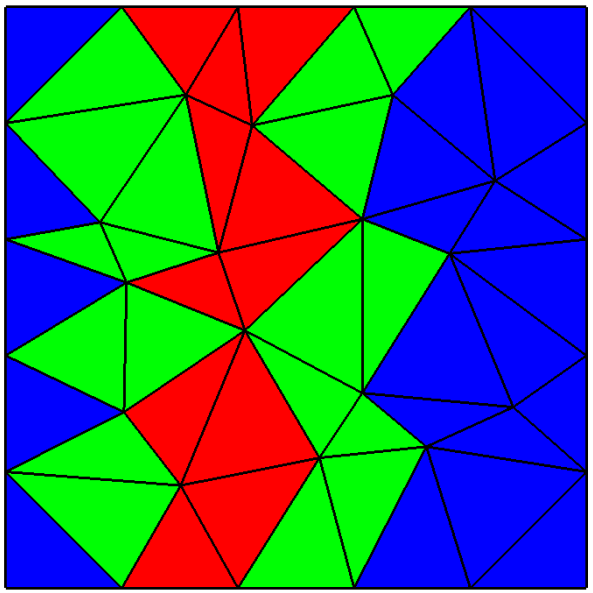

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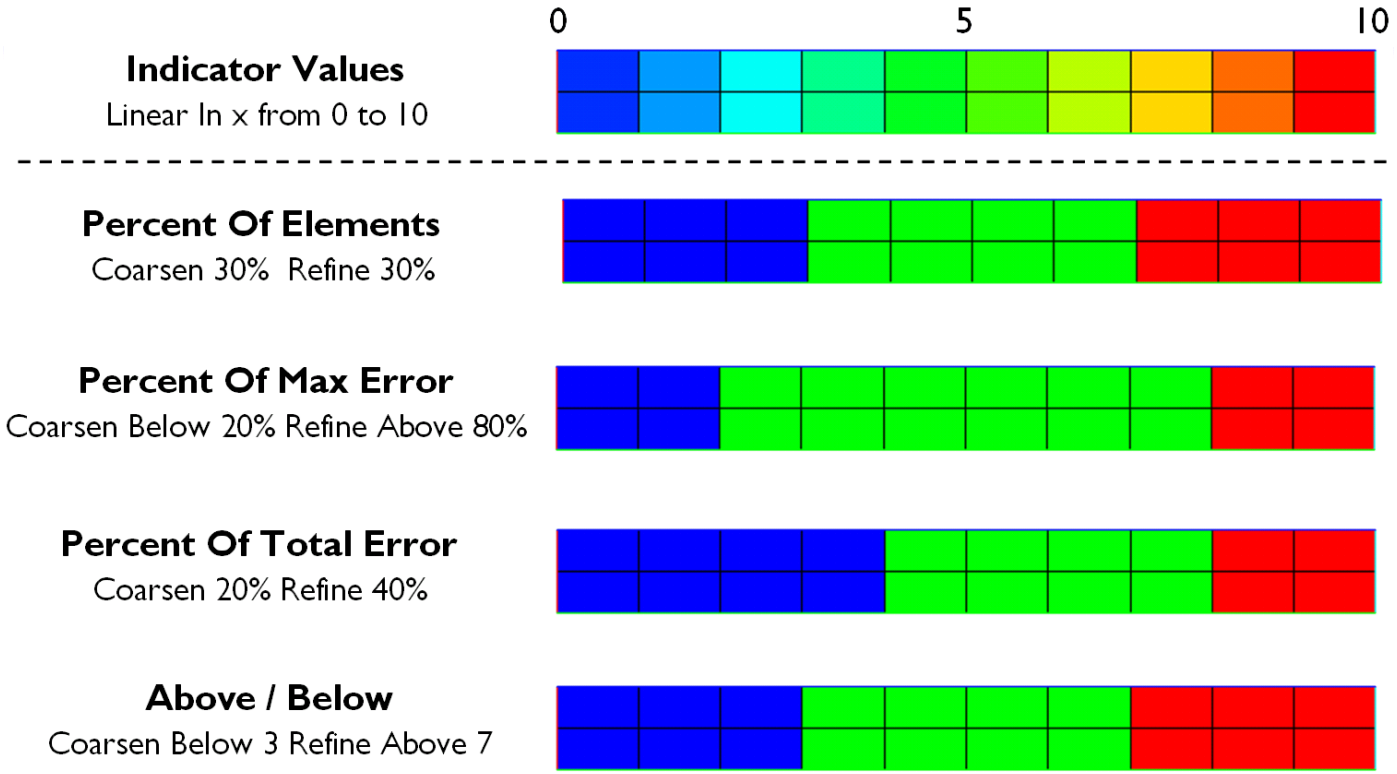

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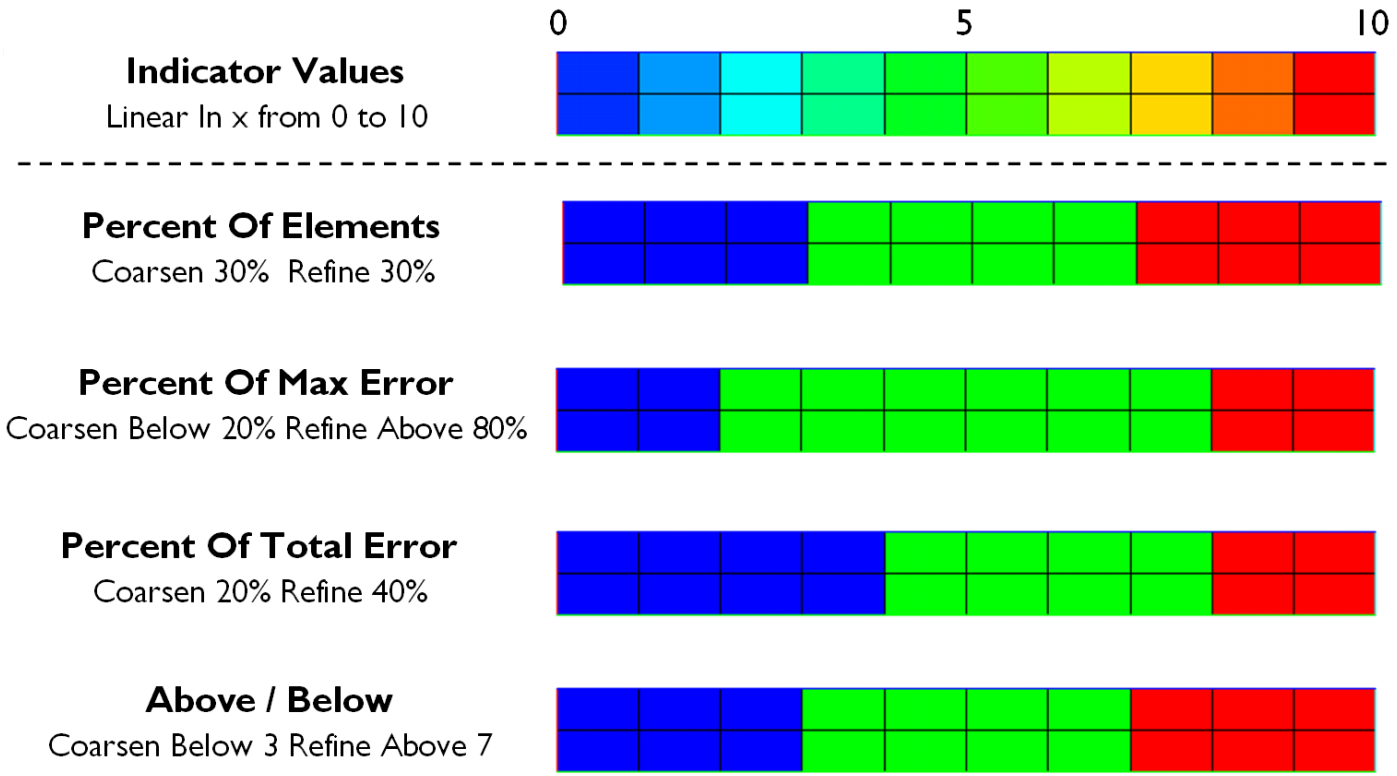

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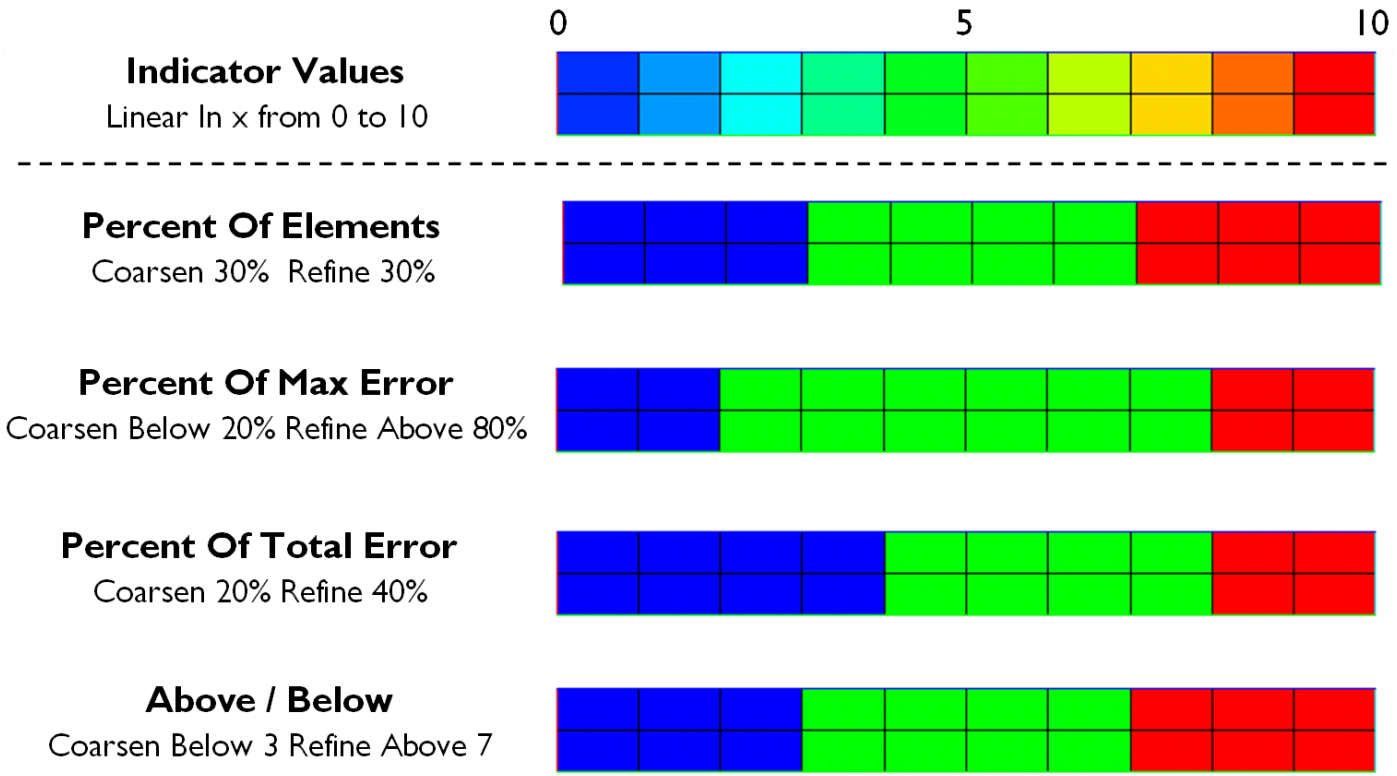

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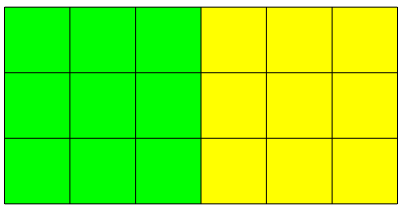
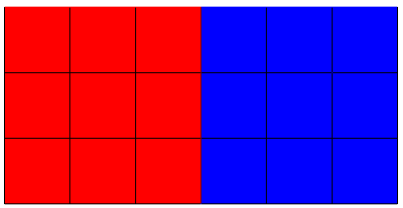


two element blocks



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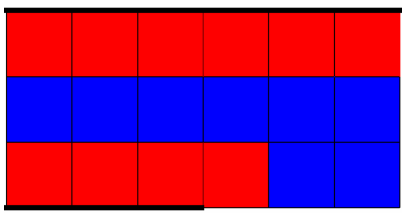

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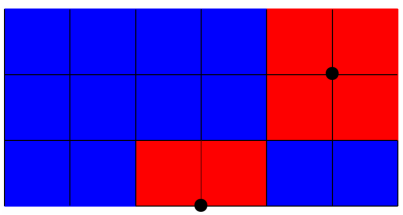

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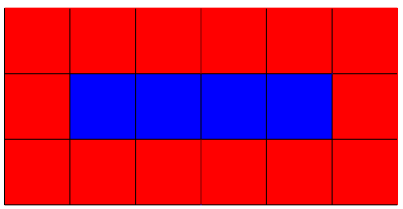
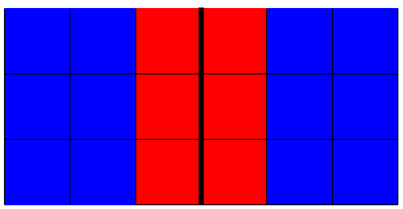


exterior boundary



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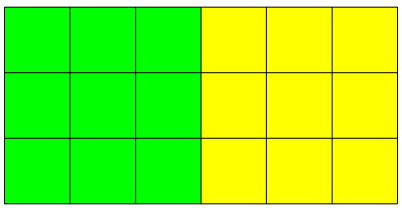

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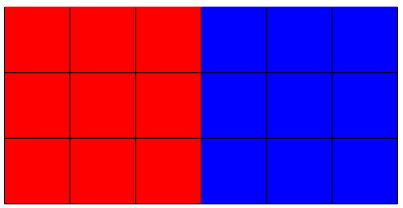

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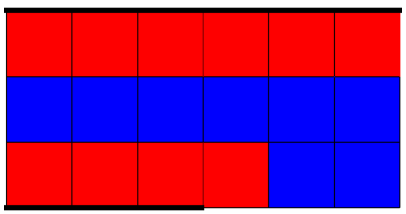

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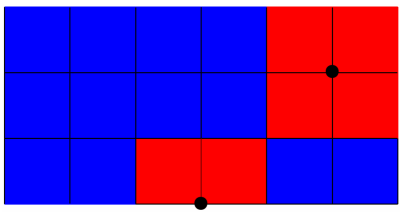

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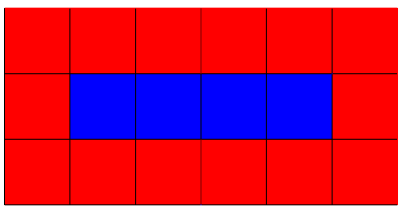

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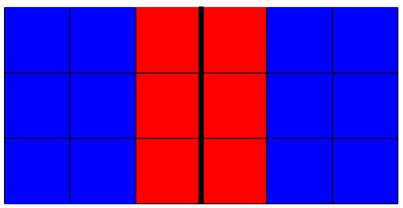

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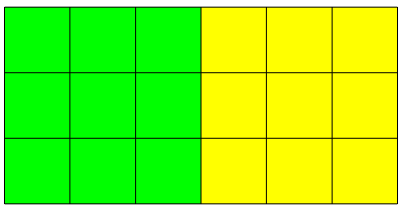

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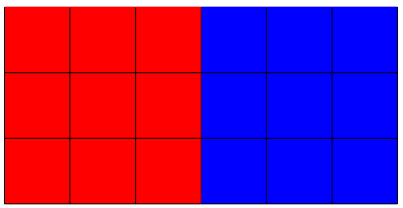

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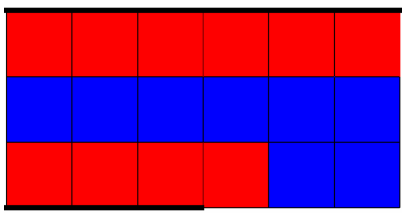

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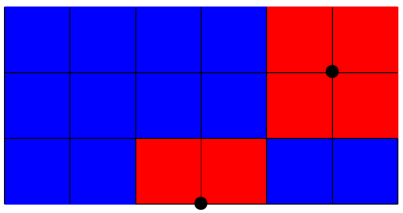

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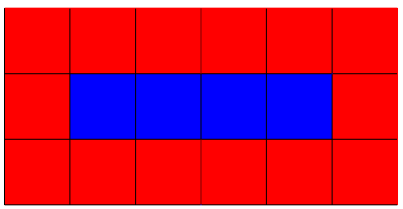

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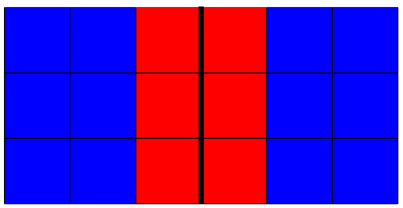

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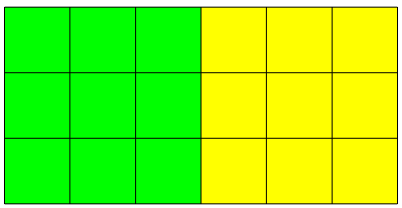

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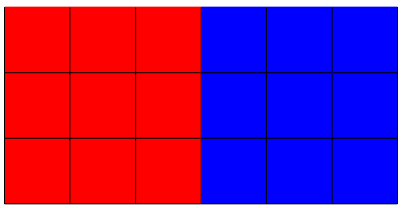
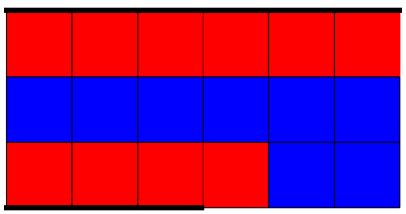


mark left block



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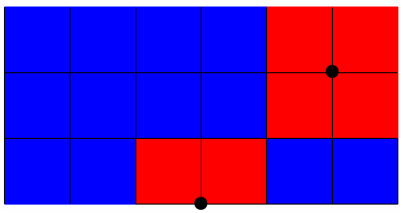

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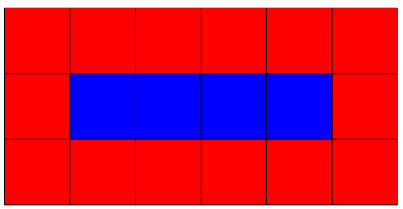
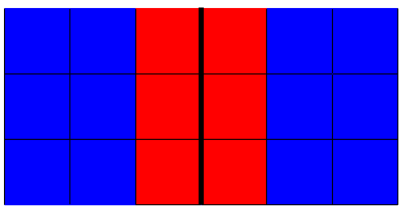


exterior boundary



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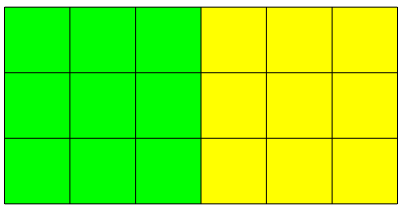

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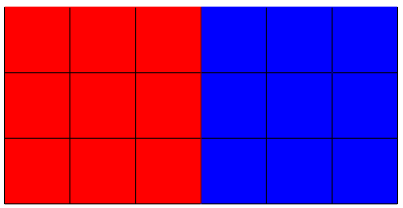

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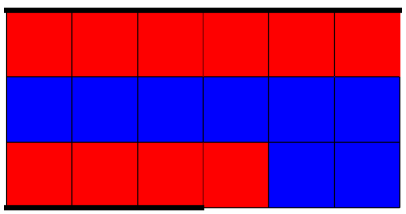

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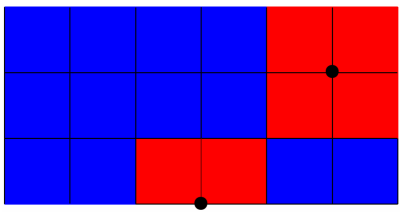

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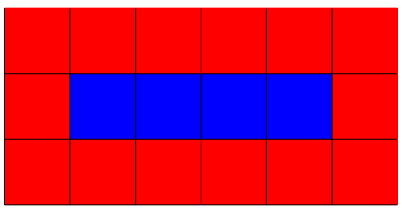

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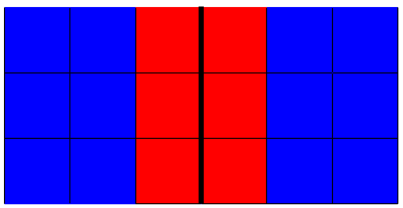

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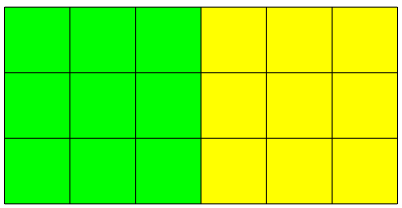

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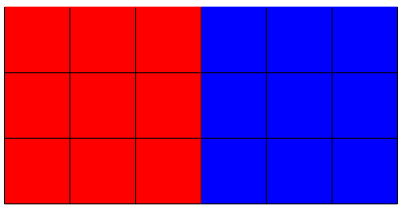

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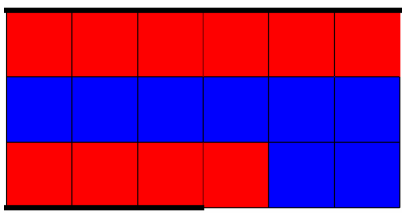

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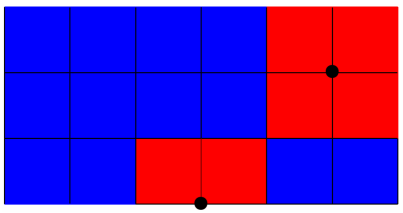

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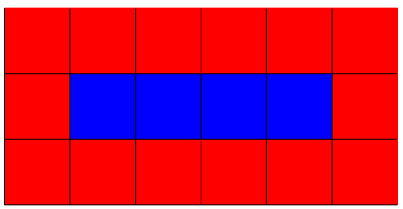

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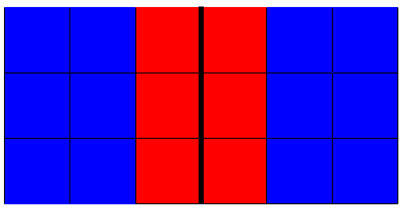

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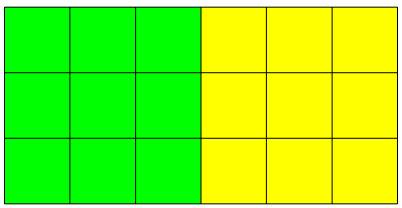

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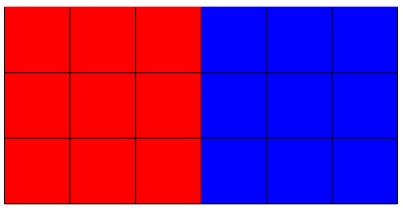

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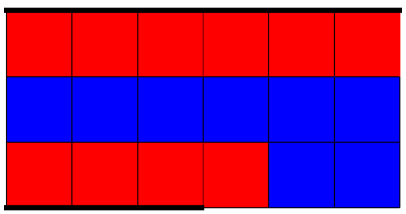

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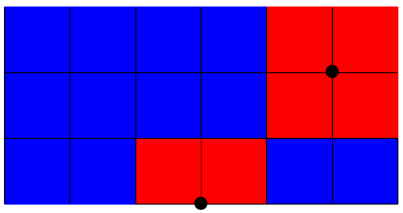

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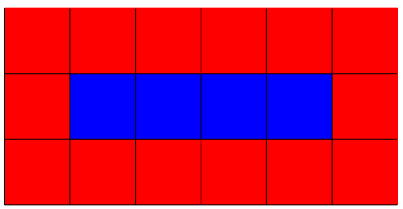

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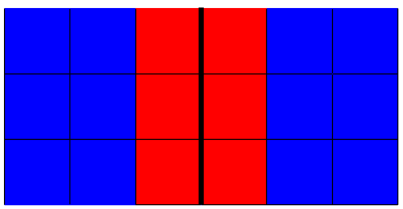

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- **Aria** is a Sierra Mechanics multiphysics code.
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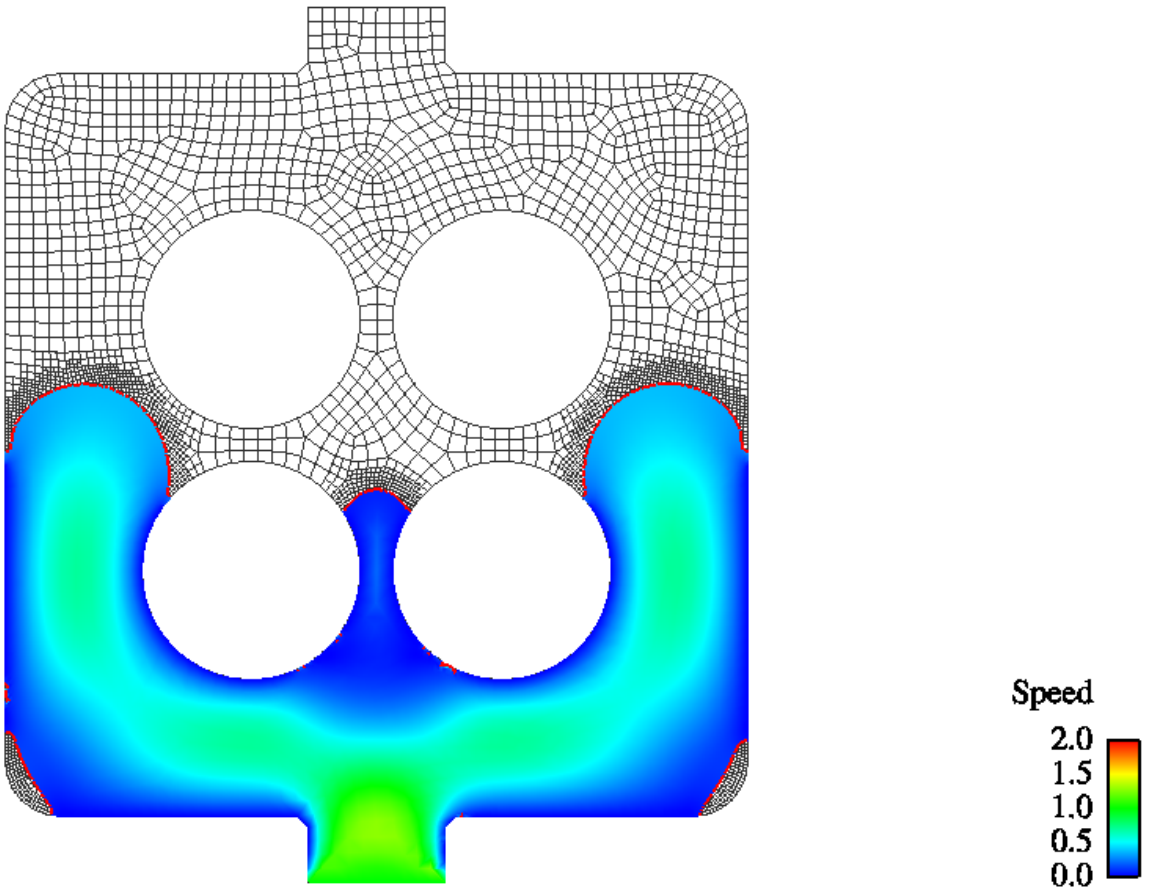
- This can be combined with error based markers.



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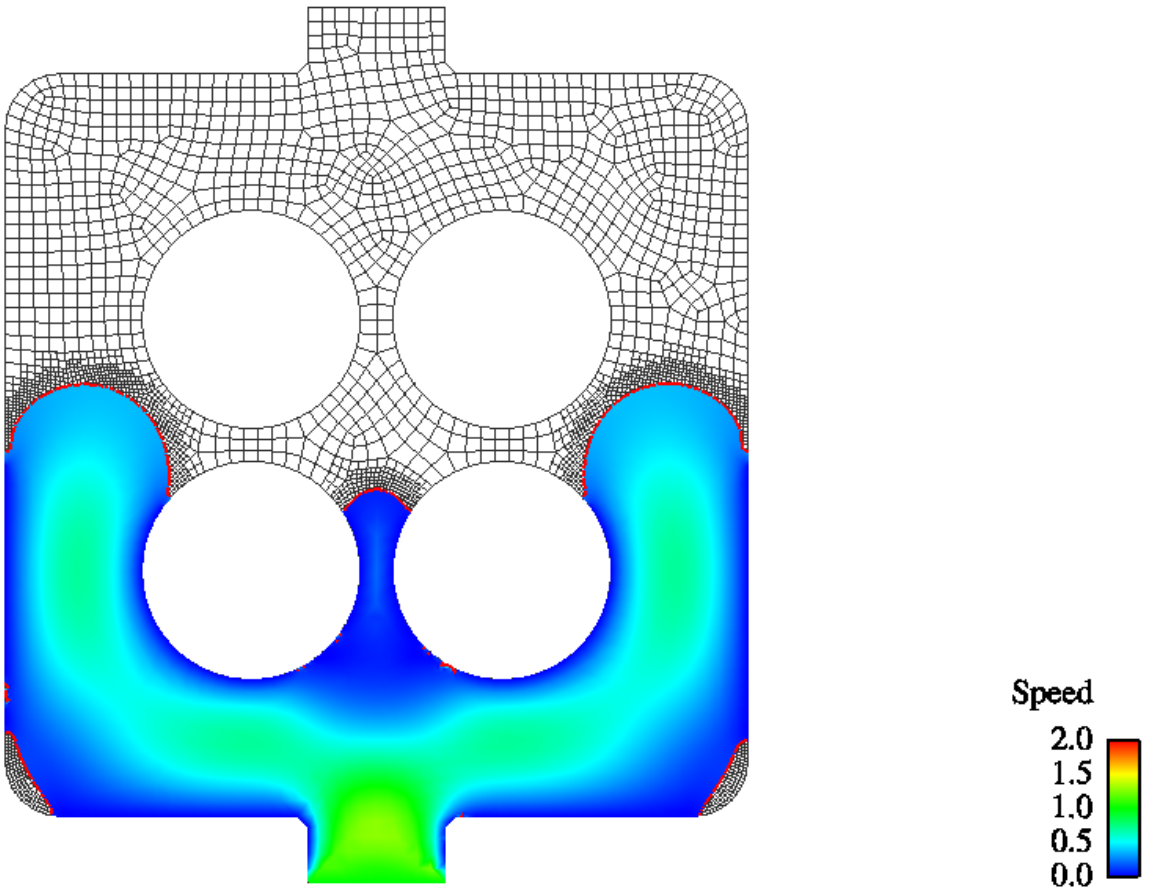

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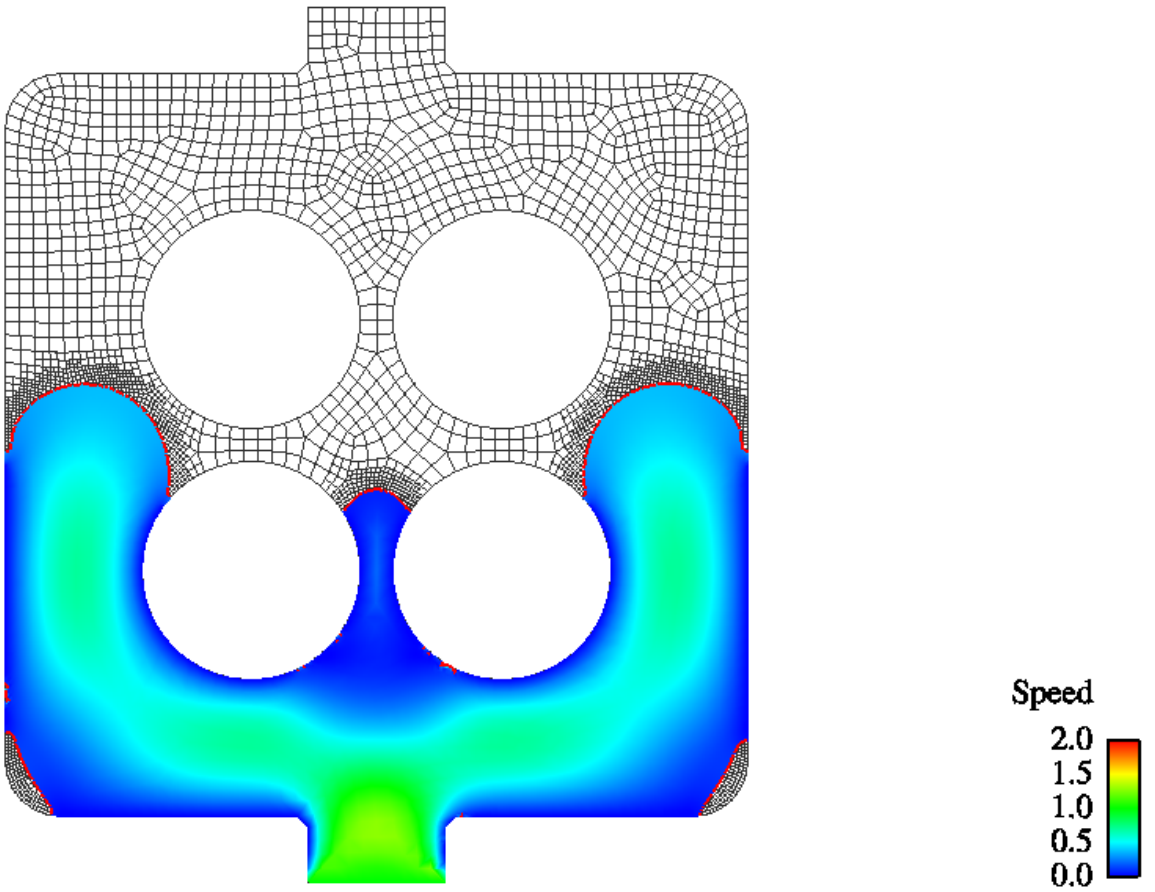

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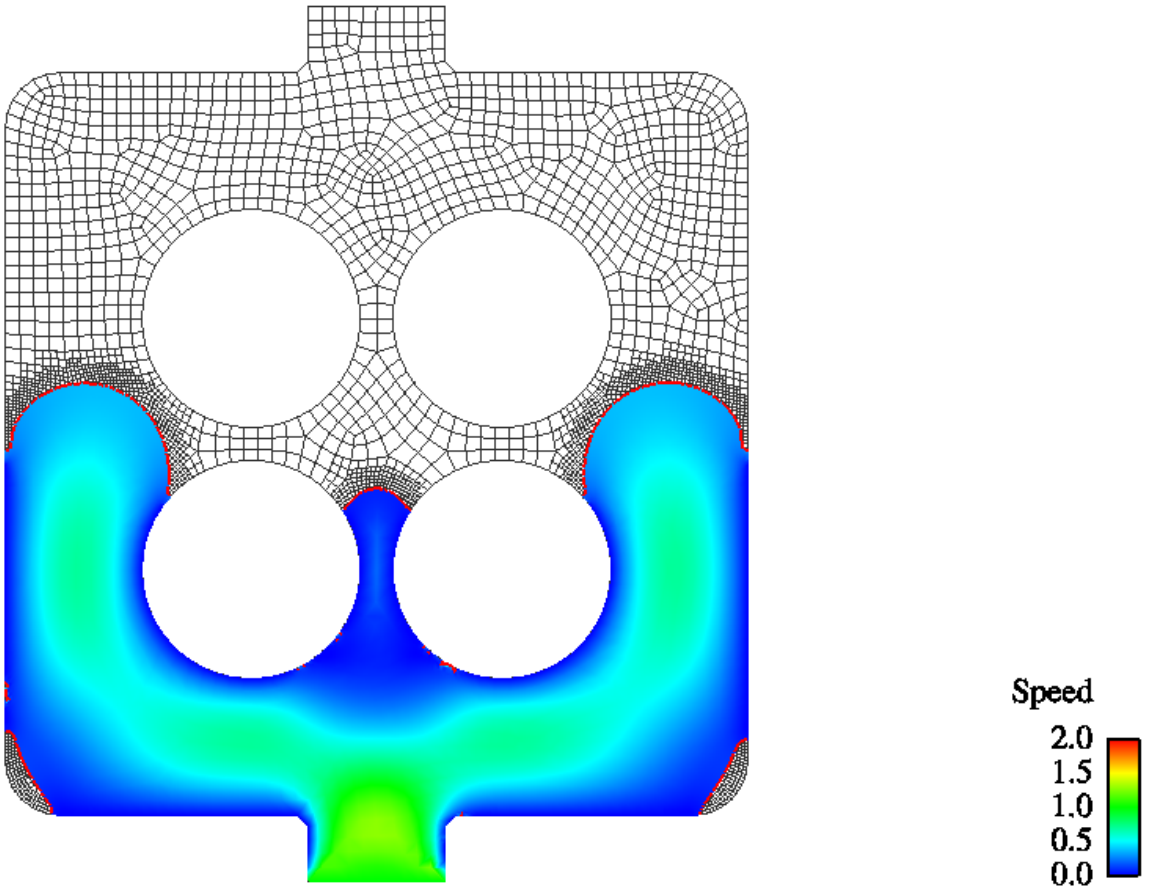

User-Driven Control of Adaptivity

- Users can gain from using error estimation and adaptivity to verify the accuracy of calculations.
- This solution verification must be reliable and easy to use.
- **Encore** has implemented an adaptivity system that is transparent, flexible, and user-driven.
- This is combined with the physics independent and adjoint-based error estimators.
- Uses of adaptivity:
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- Adjoint based error estimation for quantities of interest
- User requirements
- Linking directly to codes outside Sierra Mechanics

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