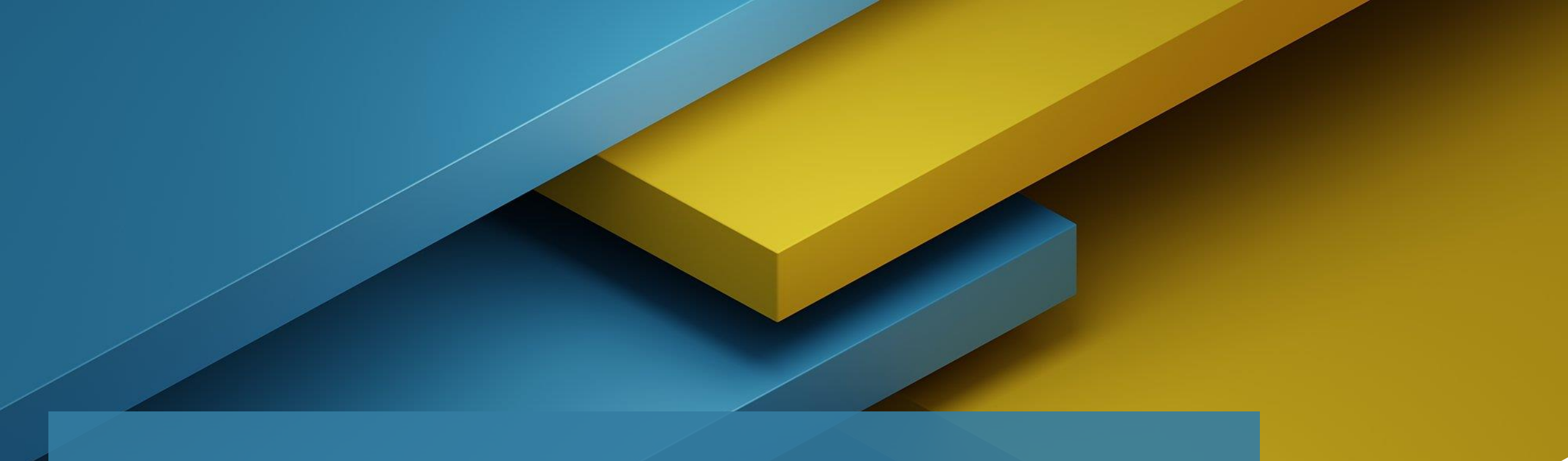

ACE+ Suite V2025.0
New Features and Enhancements

Computational Products and Solutions COE

APPLIED MATERIALS®
make possible

AGENDA

V2025.0 Features (GEOM, VisCART, ACE)

2025.0 Release Features

- GEOM
  - Improvements to Model Import
    - Enhanced CAD Import with Partial Interface Support
    - Exploded View in Selective Part Viewer
  - Improvements to Geometry Tools
    - New Size Based Entity Selection Tool
    - New Simplify Domain Tool
    - Enhanced Selected Solids Inversion Tool
    - Enhanced Solid Boolean Subtraction– Keep Tool Bodies
    - Improved Discrete Surface Splitting
    - 2D Surfaces or Rectangles from Box Creation Tool
    - Fit to Objects on Screen for Box Creation
    - Quickly Create Points on Model Surfaces
    - Interactive Draggable Objects to Geometry Tools
    - Additional Option to Place Cut Section on a Line/Curve
  - Improvements to Meshing Tools
    - Mesh Curves with # of Points and Distribution
    - Improved Quad Morphing Mesher
    - Thin Region Meshing Option Within Tet Meshing Tool
    - Interactive Draggable Objects to Several Meshing Tools
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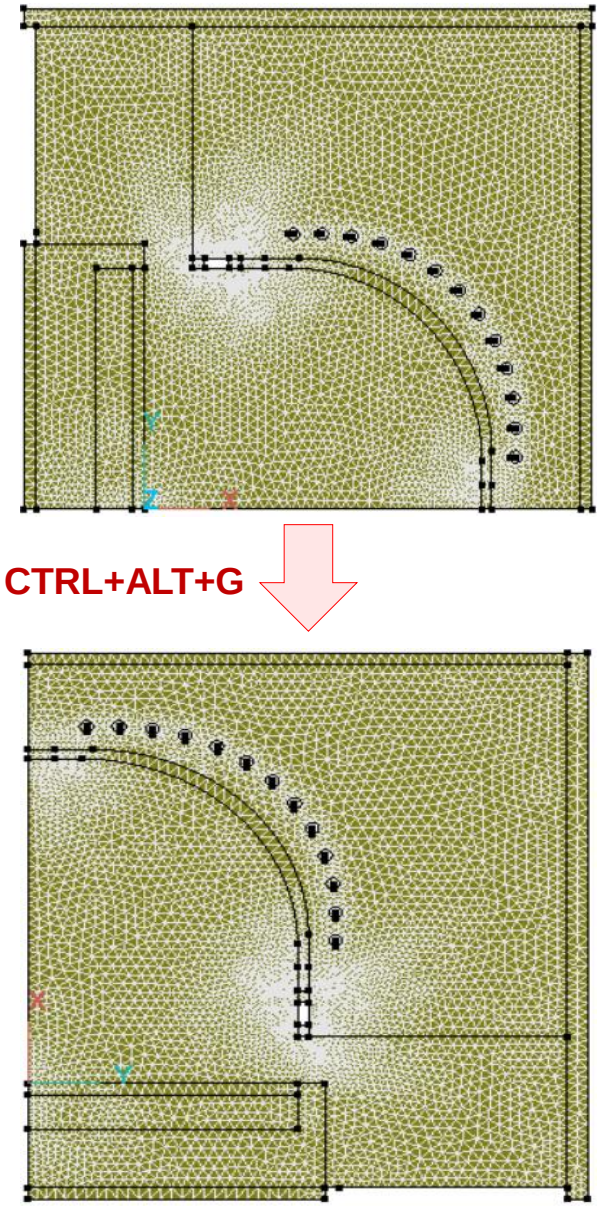
  - Search Capability in BC/VC Tools
- VisCART
  - Replace Parts with New Parts from another File
  - Patch Splitting Using Lines from Other Patches
  - Display Number of Patches for a Group or Solid
  - Interfacing Solids/Groups to Close Gaps and Prevent Mesh Creep.
  - Allow Domain Markers to Start from an Intersecting Cell in a Thin Layer
  - Measure Distance and Display Distance on Screen
  - Save STL File Command Included in Dumped VBT File
  - Mesh Quality Checks on DTF Files
- ACE+
  - Improvements to Chemistry Modeling
    - Full Stefan-Maxwell Improvements
    - Thermo-Diffusion Improvements
    - Surface Reaction Related Improvements
    - Improvements to Diffusion Calculations
  - Improvements to Plasma Modeling
    - Collisionless Monte Carlo (MCS) Support
    - Energy Bin Control for IEHD and IAHD Visualization
    - Improved Scheme to Generate Particles in Cells
    - User Specified Number of MC Particles and Iterations
    - Enhanced Particle Identification, Loading and Improved Particle Generation Process
    - MC Source Weighting Improvements

GEOM

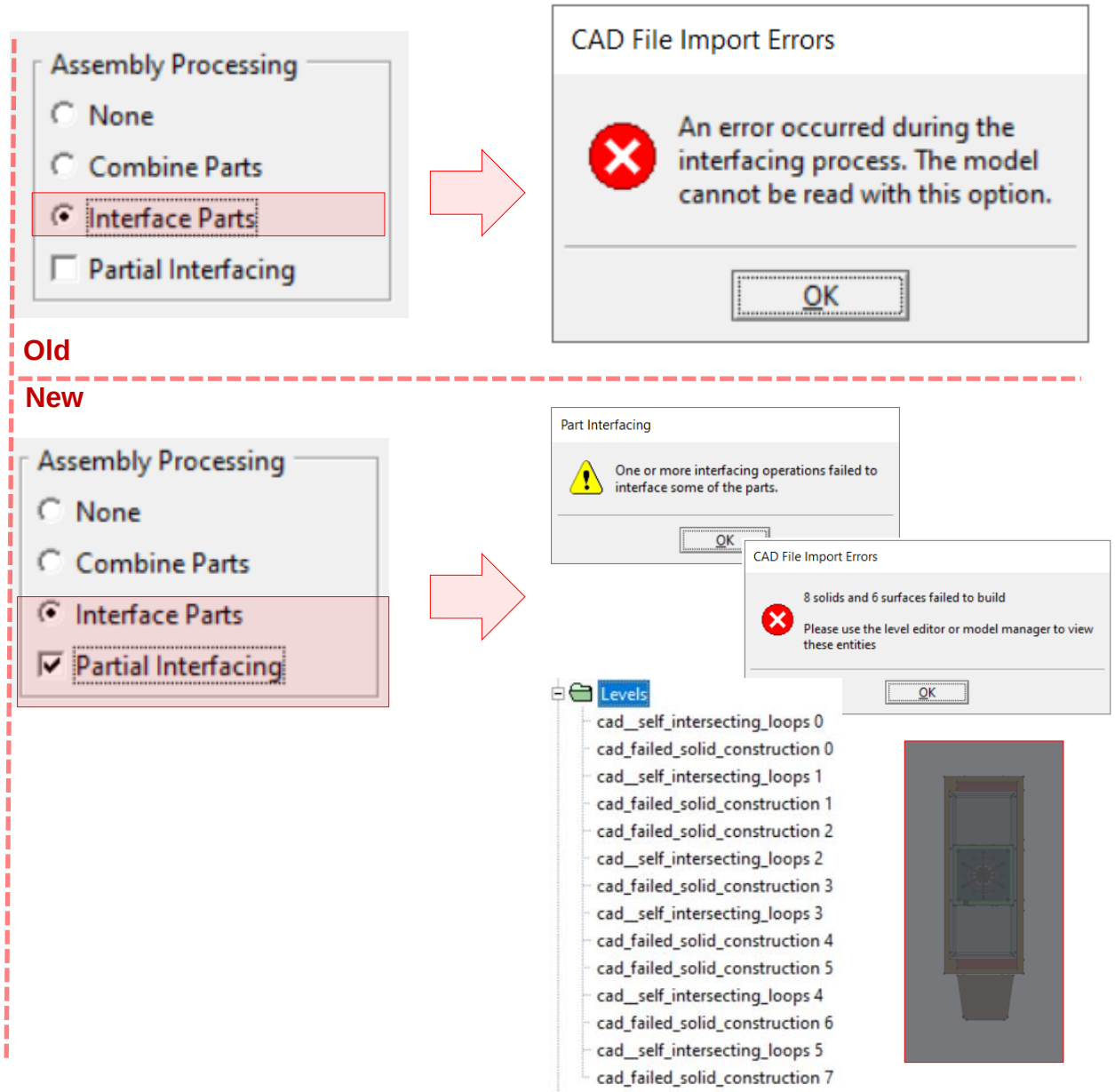
Shortcut for Axisymmetric View in GEOM

- Issue
  - » ACE uses x-axis as the axis of symmetry
  - » Engineers are used to seeing axisymmetric models with the axis on the left vertical line
  - » User has to perform multiple steps to orient the model to their preferred mode
- Enhancement
  - » A keyboard shortcut is now available to switch to this view
  - » **CTRL + ALT + G**
- Usage Guidelines
  - » Only a visualization aide
  - » Keeping model on positive x results in visual as shown in the image



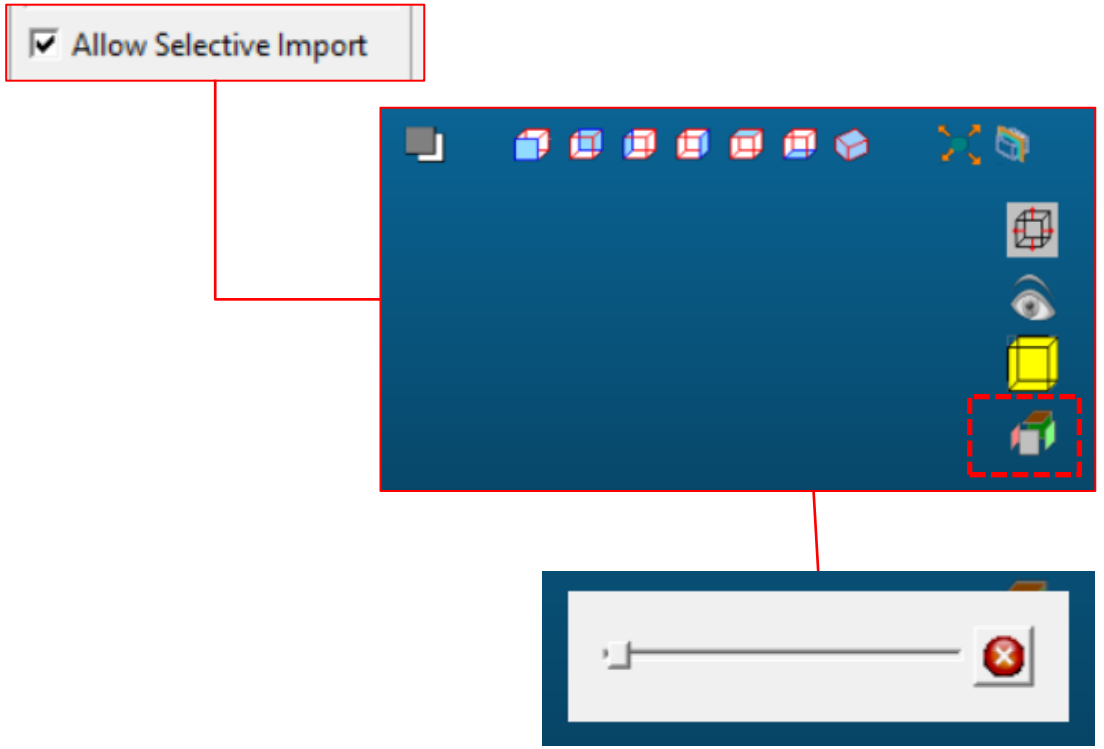
CAD Import with Partial Interfacing

- Issue
  - » CAD import with parts interfacing sometimes fail
  - » Failure results in no CAD data being imported
  - » Often, only few parts in a model fail to interface
- Improvement
  - » GEOM now supports partial interfacing
  - » Retains parts that interfaced correctly even when full interfacing fails
- Usage Guidelines
  - » “Partial Interfacing” checkbox becomes active only when “Interface Parts” is selected
  - » Use Levels in model tree to check and correct parts that failed to interface
  - » SAT and STEP formats are recommended over Parasolid for a smoother CAD import experience in GEOM



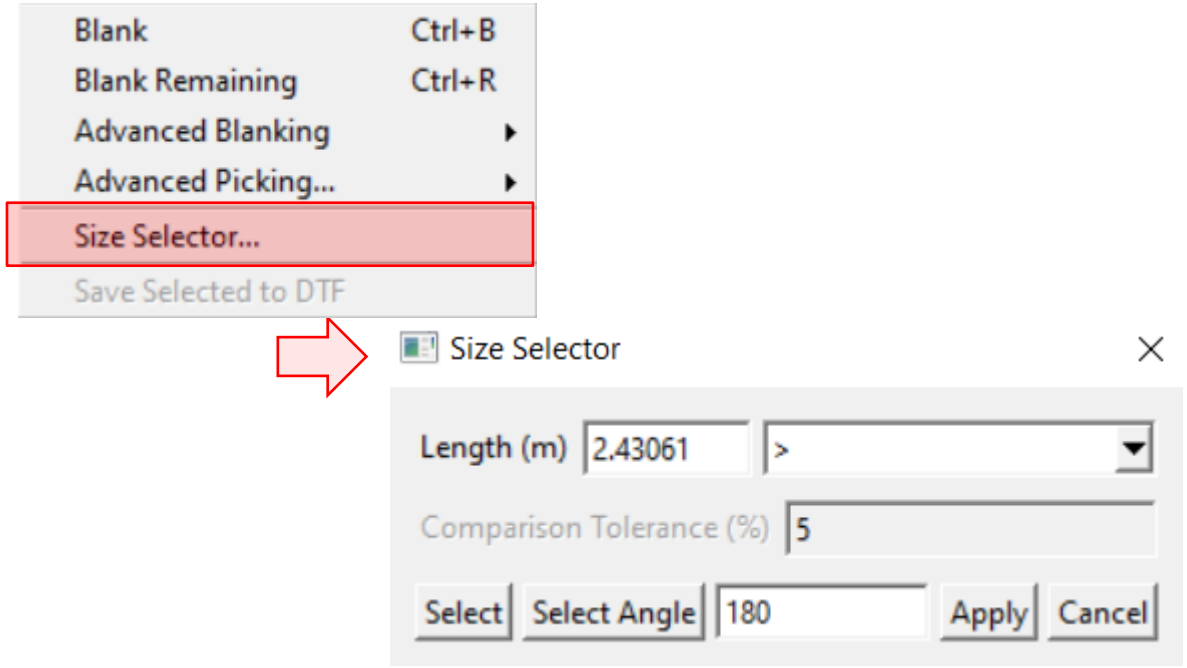
Exploded View in Selective Part Viewer

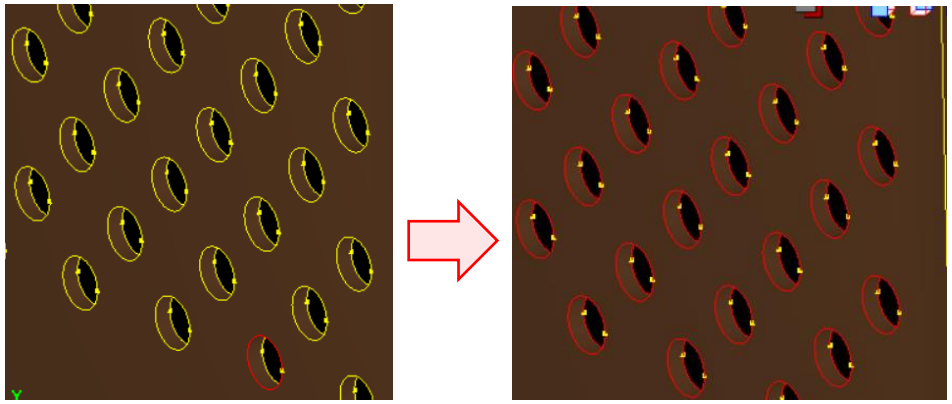
- Issue
  - » Difficult to visualize internal components without hiding
  - » Difficult to select internal components for import
- Improvement
  - » GEOM now supports exploded view in the selective parts viewer
  - » Control explosion distance for better clarity
- Usage Guidelines
  - » Use when examining assemblies with overlapping components



Size Based Entity Selection Tool

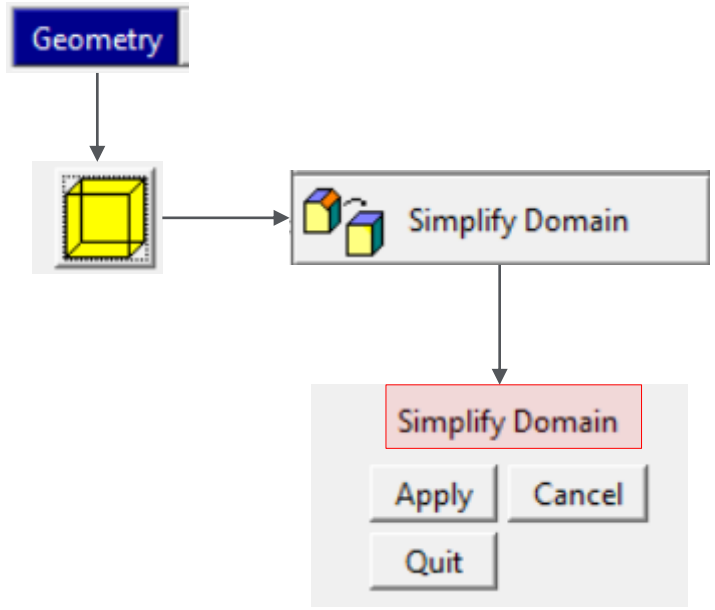
- Issue
  - » CAD models may contain numerous parts / features / entities
  - » Difficult to select such entities manually
  - » Need a selector based on size or adjacency
- Enhancement
  - » New “Size Selector” tool
  - » Works on entities with length, area or volume
  - » Different operators (==, >, <, >=, <=)
  - » Comparison tolerance (%)
  - » Iterative selection
  - » Angle based adjacency
- Usage Guidelines
  - » Select a single entity and right click to access tool

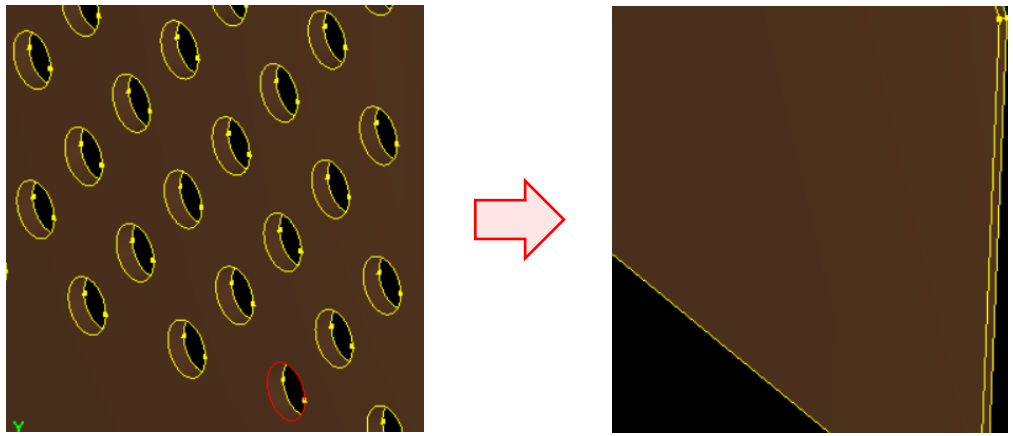




Simplify Domain

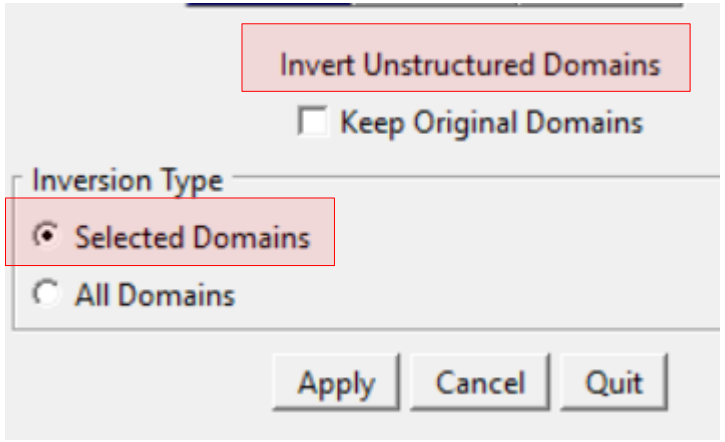
- Issue
  - » CAD models may have holes, embossments that are not necessary for modeling
  - » Need an easier tool to quickly remove such features
- Enhancement
  - » New Simplify Domain tool to remove unnecessary features (from modeling perspective)
- Usage Guidelines
  - » Use in conjunction with the size selection tool for efficiently removing small / unnecessary features





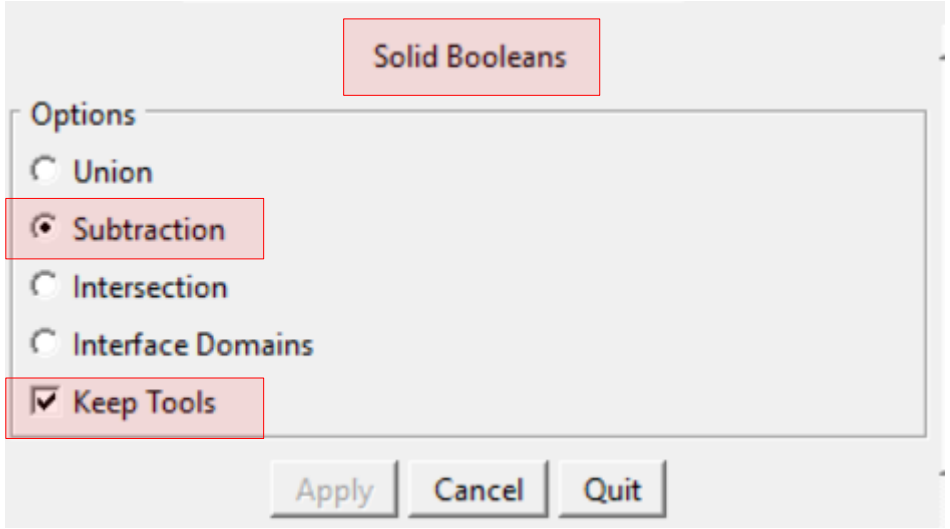
Enhanced Selected Solids Inversions

- Issue
  - » Model inversion on selected solids does not allow to remove original solids
- Enhancement
  - » The “Invert Unstructured Domains” tool now allows to keep or delete original domains upon successful inversion
- Usage Guidelines



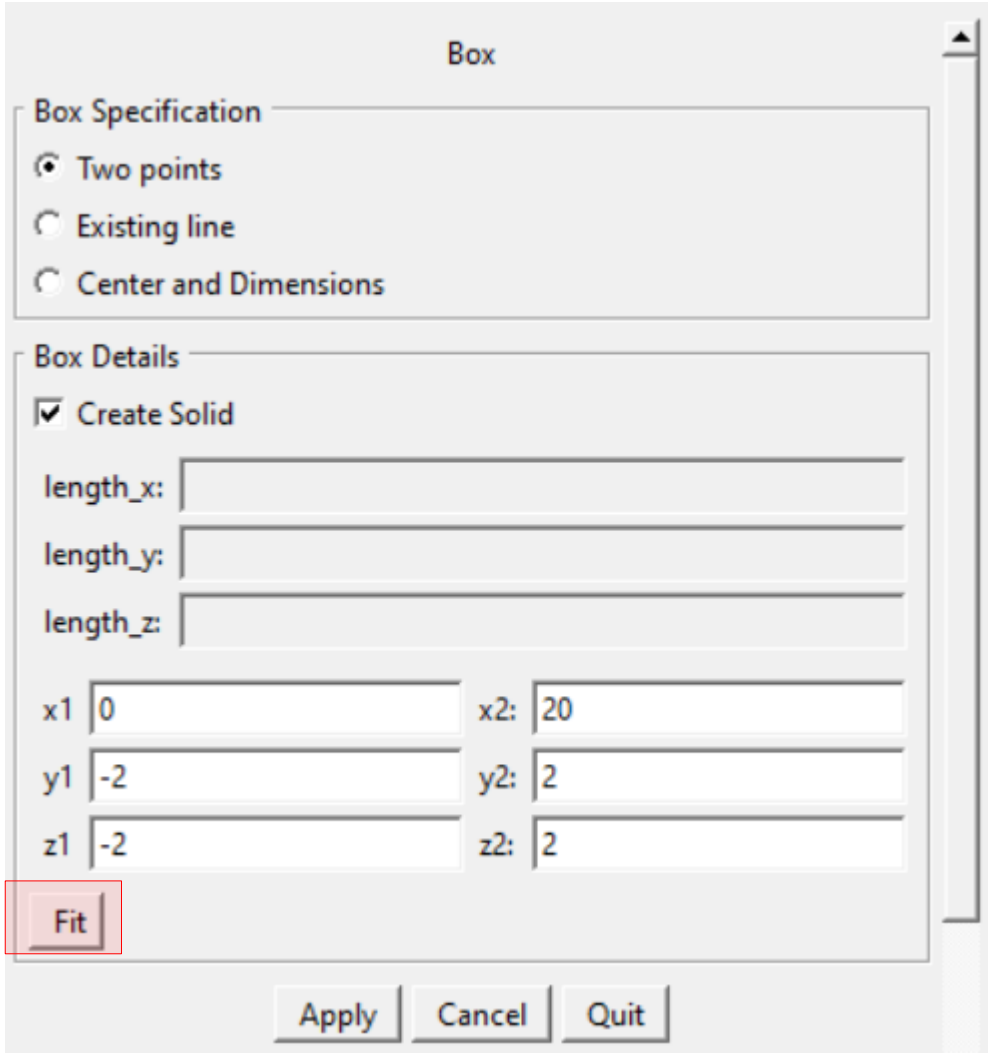
Enhanced Solid Boolean Subtraction (Keep Tool Bodies)

- Issue
  - » When performing solid Boolean subtraction, the tools (original components / solids) are removed
  - » Retaining them may be useful in some situations (e.g., Conjugate heat transfer)
- Enhancement
  - » Solid Boolean Subtraction now allows to keep tools
- Usage Guidelines



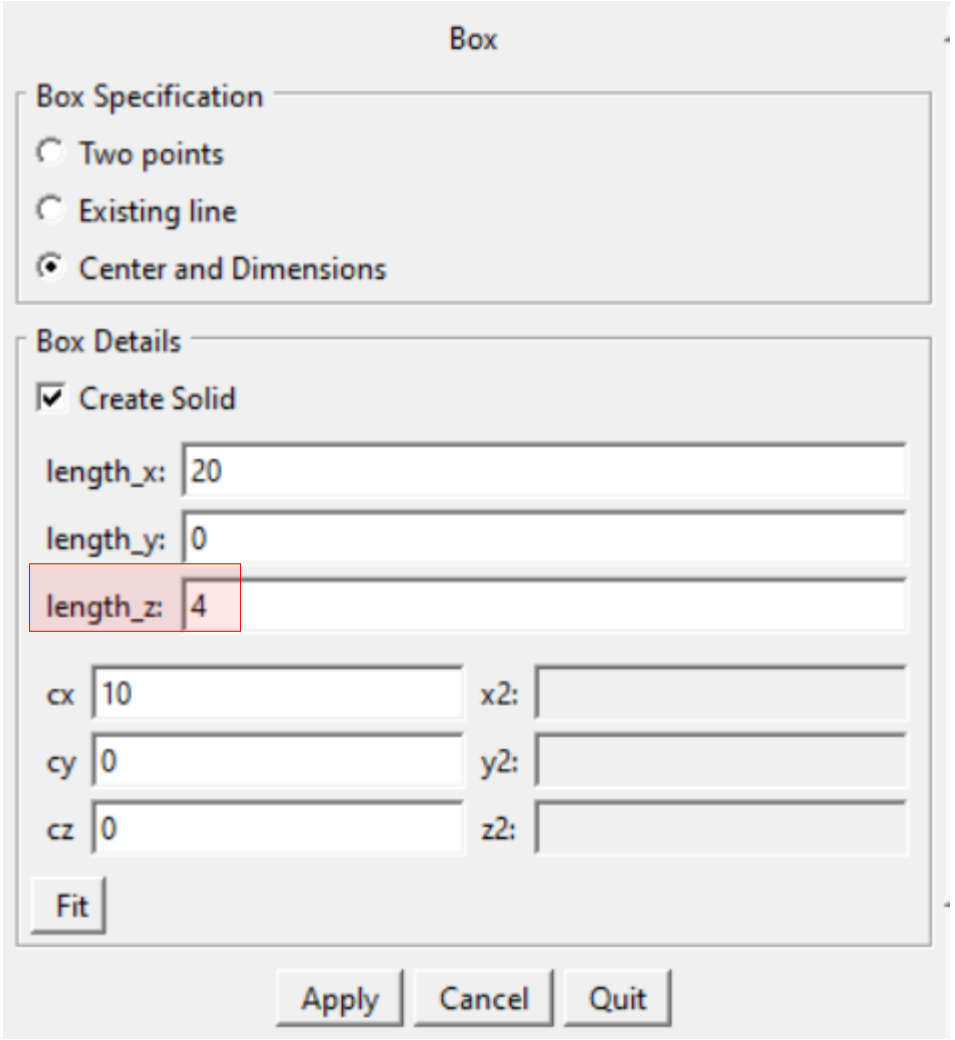
Fit to Objects on Screen for Box Creation

- Issue
  - » Box creation tool allows to create boxes in multiple ways
  - » It would be easier if user can fit a box to existing objects in the model
- Improvement
  - » A “Fit” button allows to fit a box automatically to existing objects
- Usage Guidelines
  - » This tool fits a box only to visible objects
  - » Hide other objects where you don’t want the box to extend



Create 2D Surfaces or Rectangles from Box Creation Tool

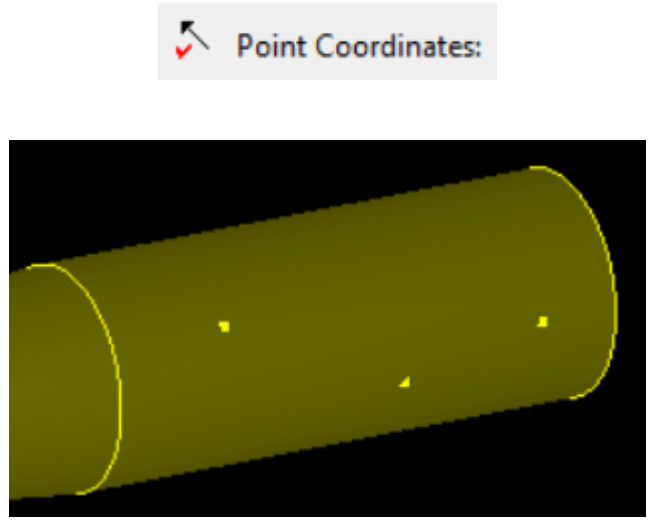
- Issue
  - » GEOM allows to create 3D box
  - » Doesn’t allow to create 2D boxes
- Improvement
  - » GEOM now allows to create 2D boxes when one of the dimension is set to 0
- Usage Guidelines
  - » Primarily intended for 2D/2D axisymmetric models such as those in plasma problems



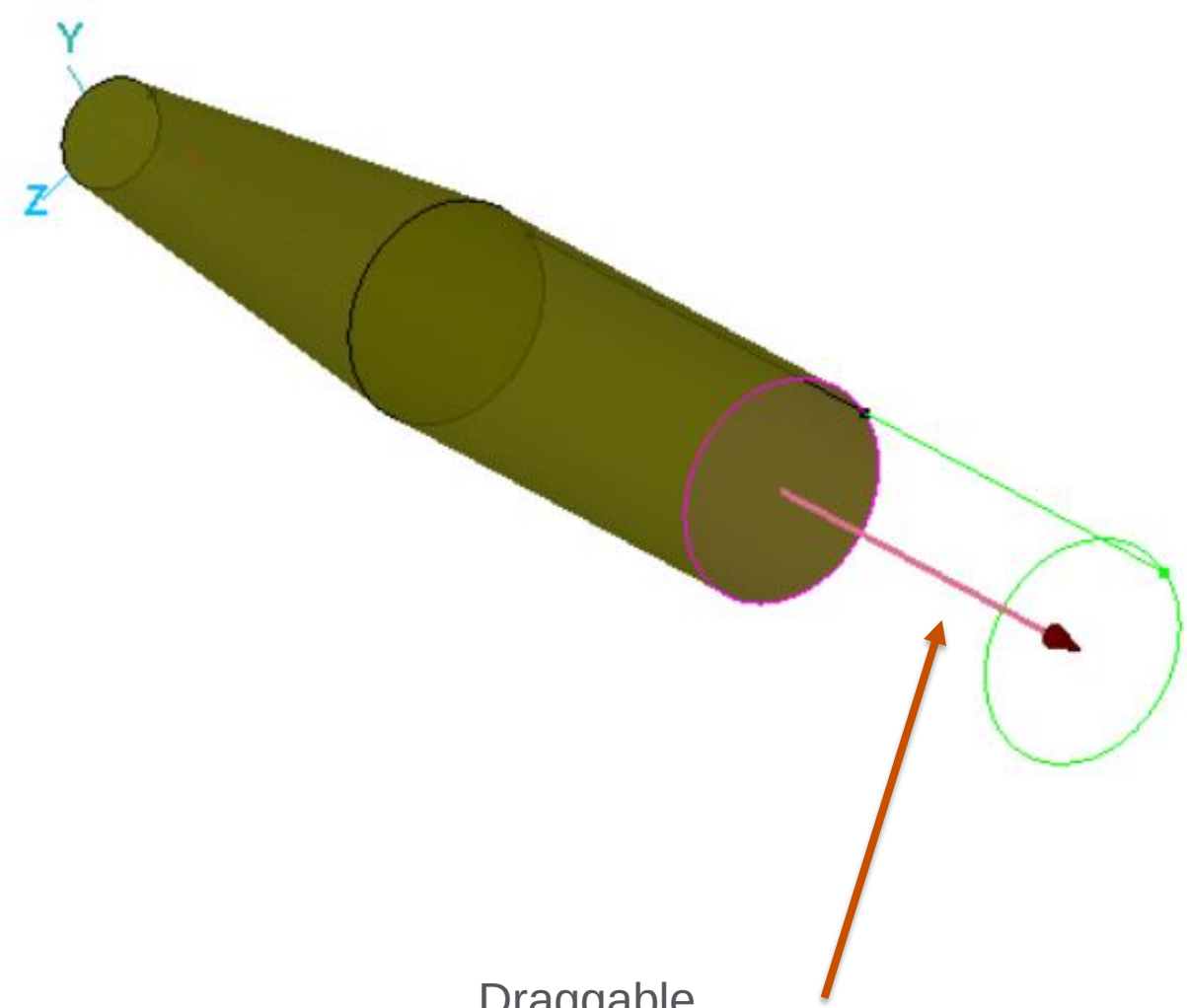
Create Points on Model Surfaces

- Improvement
  - » In certain point/line/curve creation mode the user can click on a location on a trimmed/discrete surface to create a point when the **Point creation at mouse is toggled on.**

- Usage Guidelines
  - » If the click location is such that it intersects both the current construction plane and a model location then the location closest to the eye point in the viewer will be chosen.

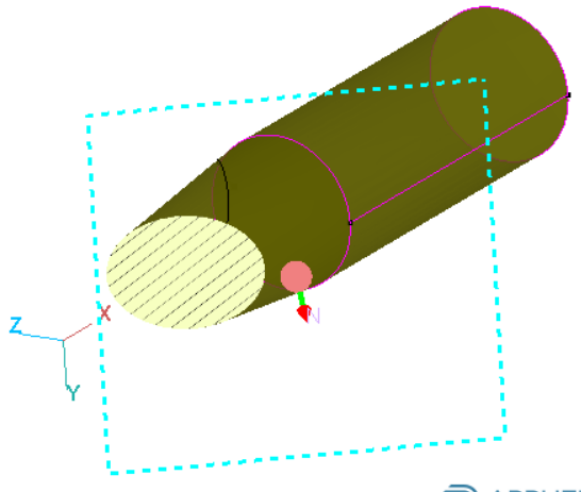


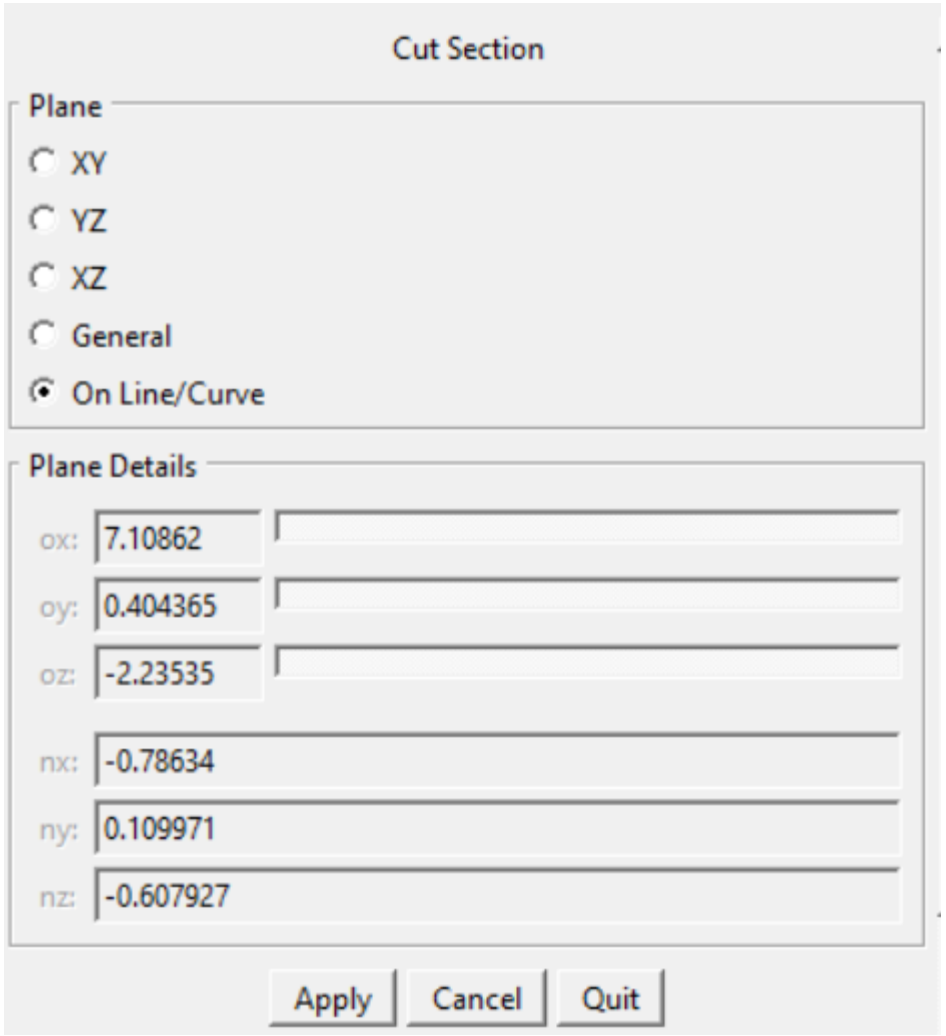
Interactive Draggable Objects to Several Geometry/MeshingTools



Option to Place Cut Section on a Line/Curve

- Usage Guidelines
  - » Click on any line or curve
  - » Cut section plane will be positioned at the click location and be oriented normal to the line or curve.



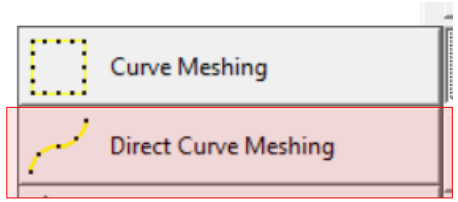


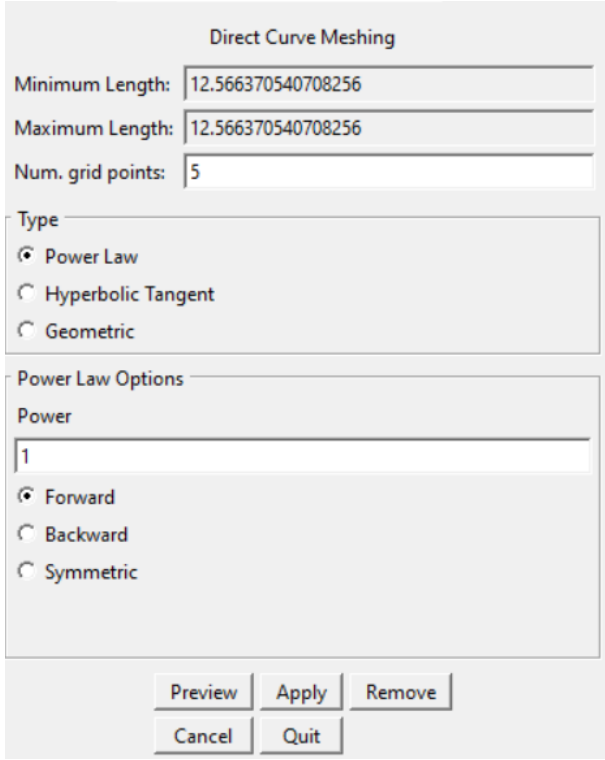
Mesh Curves with Prescribed Number of Points and Distribution

- Issue
  - » While doing unstructured mesh, users use edges to control mesh size and distribution
  - » This brings in several limitations

- Enhancement
  - » GEOM now allows to control mesh size and distribution directly on curves and lines through the Direct Curve Meshing tool
  - » All options available in edges are available now through this tool for unstructured meshes

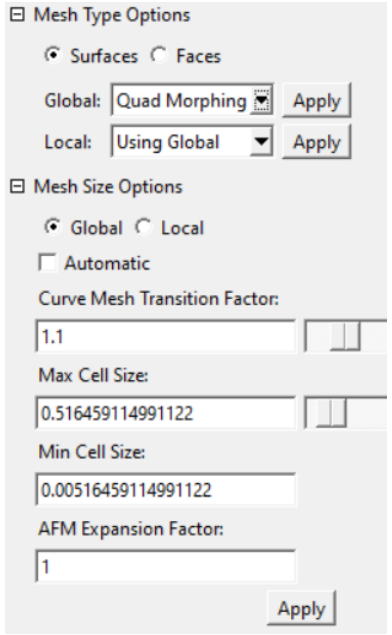
- Usage Guidelines

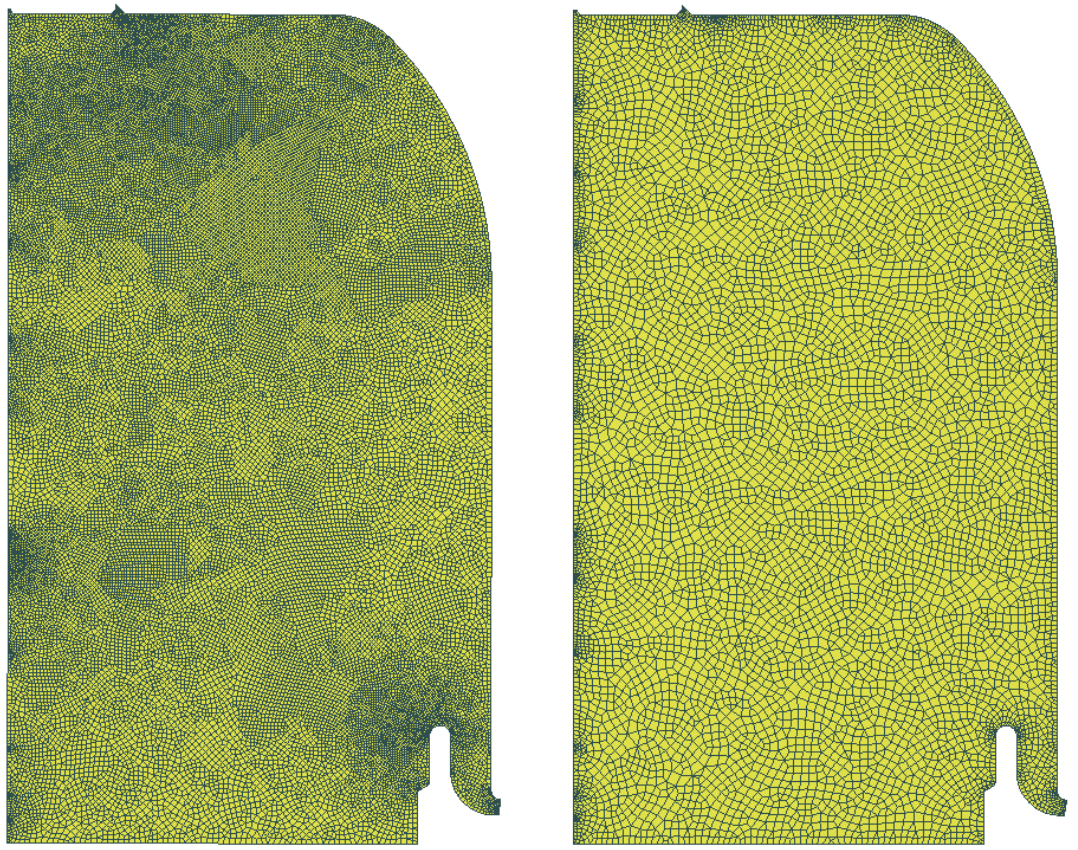




Improved Quad Morphing Mesher

- Improvement
  - » Quad morphing mesher now uses AFM instead of Delaunay for the base mesh, which allows higher quality mesh and reduced mesh count
  - » The AFM Expansion Factor allows users to control how rapidly the mesh size grows from the boundaries to the interior, allowing reduced number of cells



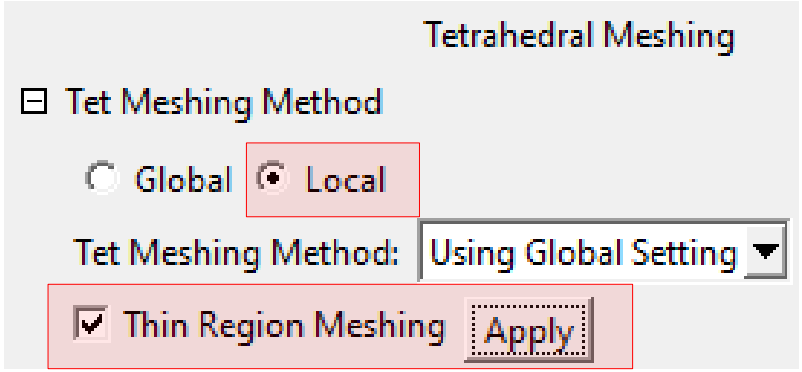


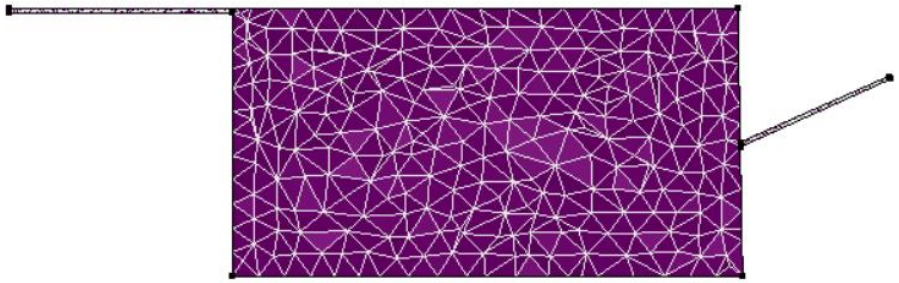
Old

New

New Thin Region Meshing Option Within Tet Mesher

- Issue
  - » Thin regions require fine surface mesh to have more than one cell (within the thin region) and thus capture gradients that may exist
  - » Need a tool to guarantee at least two cells within the thin region without over-resolving the surface mesh or the volume mesh
- Improvement
  - » A new optional processing of thin gaps is added to the tetrahedral mesh tool
  - » When selected for one or multiple volumes, it will ensure at least two tetrahedrons are generated in thin gaps
- Usage Guidelines
  - » Does not completely remove the need to refine surface mesh (users need to verify that the cells are not too flat and thus have solver issues)

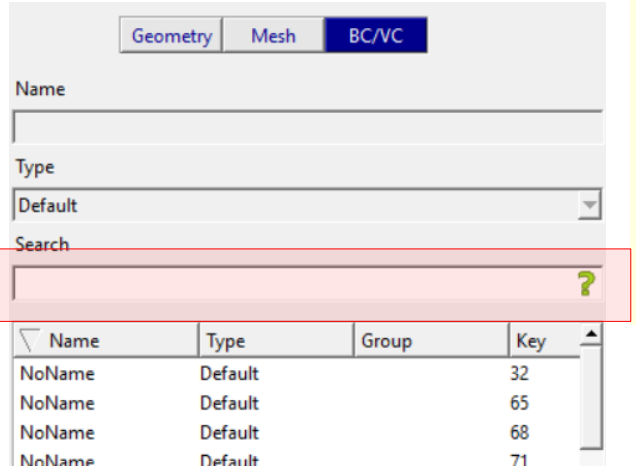




Search Capability for BC/VC Tools

- Issue
  - » Large models may have 100s or 1000s of VCs and BCs
  - » Difficult to scroll and find an object of interest

- Enhancement
  - » A search tool is now available in the BC/VC section



Search terms are NOT case-sensitive.

Multiple, space-delimited search terms can be specified.

By default, only boundary conditions that match ALL search terms are found.

You can use the following operators to refine the search:

`-` A dash can be used to exclude a search term from the search.
`-type:wall` (find all boundary conditions except walls)

`or` OR can be used to indicate optional search terms.
`type:inlet or type:outlet` (find all inlets and outlets)

`"` Quotes can be used to specify a search term that contains a space.
`name:"My Box"` (find boundary conditios whose name contains "my box")

`name:` Searches only names for the given term.
`name:inlet` (find boundary conditios whose name contains "inlet")

`type:` Searches only boundary condition types for the given term.
`type:wall` (find all walls)

`group:` Searches only boundary conditions under the given group.
`group:grp_1` (find all boundary conditions in group with name=grp_1)

VisCART

2025.0 Release Features

- GEOM
  - Improvements to Model Import
    - Enhanced CAD Import with Partial Interface Support
    - Exploded View in Selective Part Viewer
  - Improvements to Geometry Tools
    - New Size Based Entity Selection Tool
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    - MC Source Weighting Improvements

Mesh Quality Checks on DTF Files

- CFD-VisCART (from command line)
  - » -check_dtf_q <dtf_file>
  - » Added in the command line to check and display grid quality
  - » Simulation is assumed to be 1.
- In batch mode
  - » check_dtf_quality dtf_file sim# to do the same test.
- In python script
  - » check_dtf_quality(dtf_file, sim#)
- Works only for 3D meshes

```
                                CFD-VisCART -check_dtf_q test_arb_interf_rotation
.DTF
**************Current Volume Mesh Quality Report**************
|                                        Number of Cells:                                14000 |
|                                  Negative Volume Cells:                                    0 |
|                     Large Volume Ratio Cells (>100.0):                                     0 |
|                                  Maximum Volume Ratio:                                  1.33 |
|                                      Degenerate Faces:                                     0 |
|                     Non-Convex Cells (Skewed Angle<0):                                     0 |
|                          Skewed Boundary Faces (<5.0):                                     0 |
|                    Minimum Skewed Boundary Face Angle:                             87.40028 |
|                          Skewed Interior Faces (<5.0):                                     0 |
|                    Minimum Skewed Interior Face Angle:                             73.03336 |
|                             Smallest Skewed Angle is at:                       Interior Faces |
|             Location of the Smallest Skewed Angle Face: (-0.000722135, 0.038989, 0.000120282
) |
|             Cell Center Jumping Cells (>0.01*(vol^1/3)):                                   0 |
|                       Faces with Folding Angle > 150.0:                                    0 |
|                              Multiple Faces in Between:                                    0 |
| Cells with Multi-Adjacent BFacets (Normal Angle≤30):                                       0 |
************************************************************
```

ACE+

Multicomponent Diffusion

- Stefan Maxwell Equations

$$\sum_{J \neq i} \frac{x_i x_J}{D_{ij}} (\boldsymbol{v}_j - \boldsymbol{v}_i) = -\nabla x_i \qquad \boldsymbol{A.J = B}$$

Full Stefan Maxwell

- Wilke formula for effective diffusivity

$$D_{i,eff} = \frac{1 - x_i}{\sum_{j \neq i} \frac{x_j}{D_{ij}}} \qquad J_i = -D_{i,eff} \nabla x_i$$

Approximate SM

- Conservation of species flux

$$\sum_{k=1}^{N} J_k = 0$$

- Conservation of species mass fraction

$$\sum_{k=1}^{N} Y_k = 1$$

GUI INPUTS					WITHIN SOLVER			
Mass Diffusivity	Conservation of Species	Thermo Diffusion	Diffusivity	Species Conservation	Matrix Solve	Wilke Formula	Flux Conservation	Mass Fraction Conservation
MCD	OFF							
MCD	ON		Approx. SM	None				
MCD	ON			Reference Species				
MCD	ON		Approx SM	Normalization				
MCD	ON		Full SM	Normalization				

Improvements to Multi-Component Diffusion

- Issue
  - » Previous versions of **Full Stefan Maxwell** model used a direct matrix inversion which required very high memory and prohibitively slow for models with large number of species
- Improvement
  - » A new iterative matrix inversion is introduced which is faster for models with large number of species
  - » Defaults to the new iterative matrix inversion if the number of species exceeds 10
- Issue
  - » In previous versions**, calculations for variables like diffusivity and density** were being carried out multiple times within each iteration leading to increased computational time
- Improvement
  - » This algorithm has been modified to reduce these calculations without compromising the solution correctness
  - » Results in improved turnaround time for all multi-component

Improvements to Multi-Component Diffusion

- Issue
  - » Models with **surface reactions** didn’t converge as well as they did in previous versions
- Improvement
  - » Several changes have been made to these algorithms and the convergence issue is as good as the previous versions
  - » Primarily related to the Stefan convection term (alters the species gradient due to mass production / removal)
- Usage Guidelines
  - » No changes in GUI / setup
  - » Only performance changes

Improvements to Multi-Component Diffusion

- Turnaround time

				Approx. Stefan Maxwell			Full Stefan Maxwell		
	Mesh Type	Mesh Size	No. of Species	2024.5	2025.0	% Diff	2024.5	2025.0	% Diff
case_01	CFD-VisCART	2.2 M	9	35.72	33.91	5.07%	44.61	31.66	29.03%
case_02	CFD-VisCART	4.04 M	9	81.36	78.69	3.28%	106.83	76.48	28.41%
case_03	CFD-VisCART	0.99 M	17	6.56	6.05	7.77%	39.83	11.28	71.68%
case_04	Tetra+Prism	5.76 M	17	37.4	34.1	8.82%	229.2	71.8	68.67%
case_05	Hexahedral	0.82 M	17	8.2	7.64	6.83%	55.16	17.11	68.98%

Approximate Stefan Maxwell differences come from diffusion calculation related improvements

Full Stefan Maxwell differences come from both diffusion calculation related improvements and iterative matrix inversion

Though larger reduction in turnaround time is observed for Full Stefan Maxwell, the absolute time will still be more than Approximate Stefan Maxwell

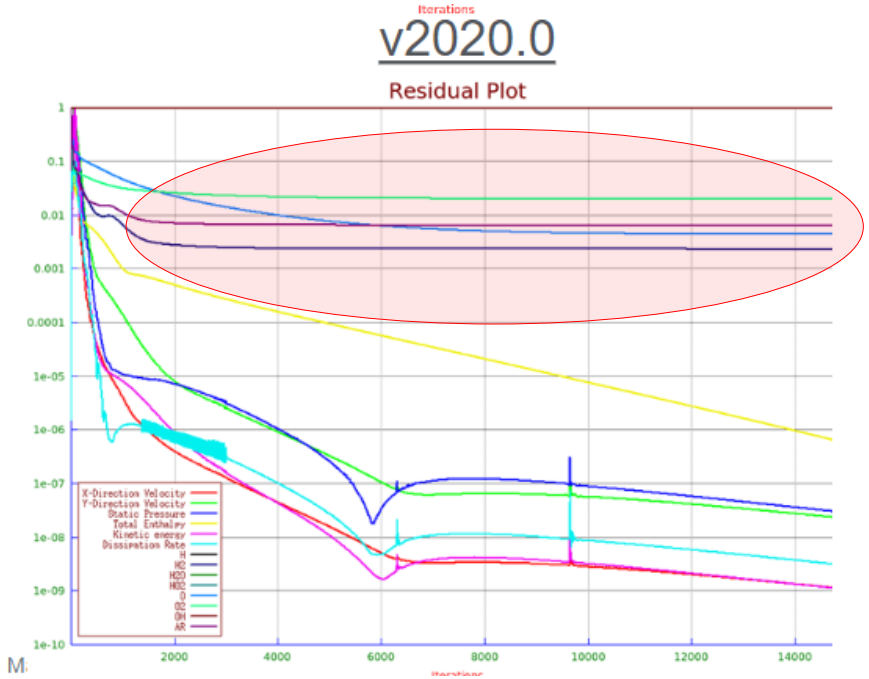
Improvements to Multi-Component Diffusion

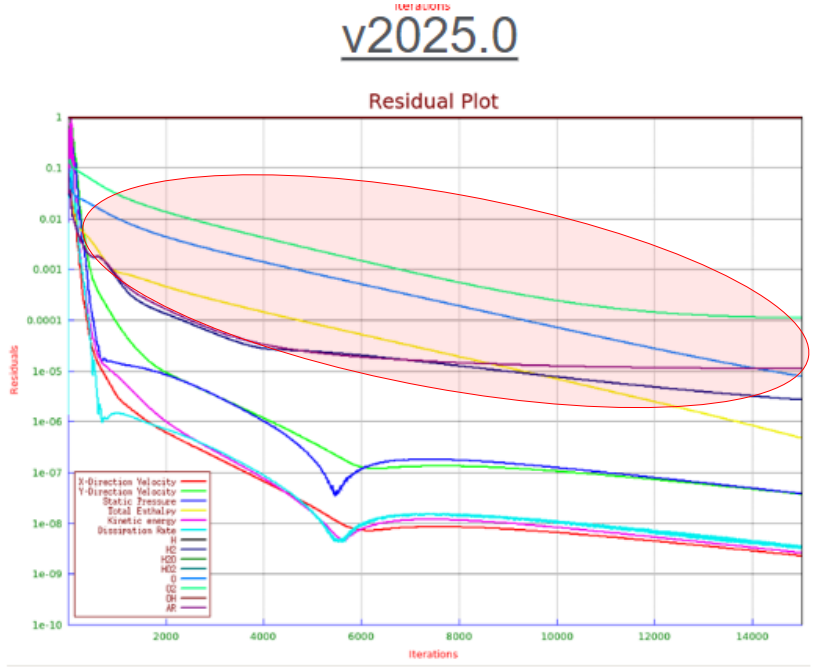
- Turnaround Time (Thermo Diffusion)
  - » All runs with ASM

	Mesh Type	Mesh Size	No. of Species	2024.5	2025.0	% Diff
case_01	2D-Quad	1500	41	0.375	0.262	30.13%
case_02	CFD-VisCART	4.04 M	12	85.05	80	5.94%
case_03	CFD-VisCART	0.99 M	41	17.18	14.29	16.82%
case_04	Tetra+Prism	5.76 M	17	37.4	34.1	8.82%
case_05	Hexahedral	0.82 M	41	10.83	9.56	11.73%
case_06	2D-Hybrid	42.87 K	8	2.38 (2019.0)	1.54	35.29%
case_07	2D-Hybrid	1184	23	88.27 (s)	90.25 (s)	-2.24%

Improvements to Multi-Component Diffusion

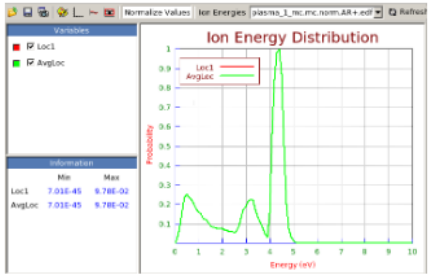
- Convergence

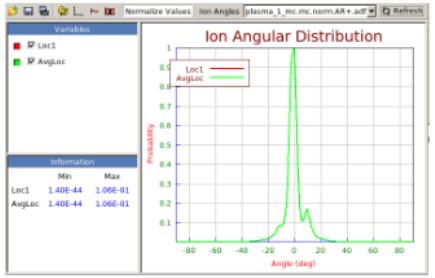




Collisionless Monte Carlo Support

- Enhancement
  - » Users can switch on or off collisions for MC-IEADF simulation
  - » Helpful to users in the following manner.
    - Provides a better insight of how collisions impact the Ion Energy Distribution Function (IEDF) and Ion Angular Distribution Function (IADF)
  - » Serves as a diagnostic tool for spatiotemporal characteristics of MC particles and sheath





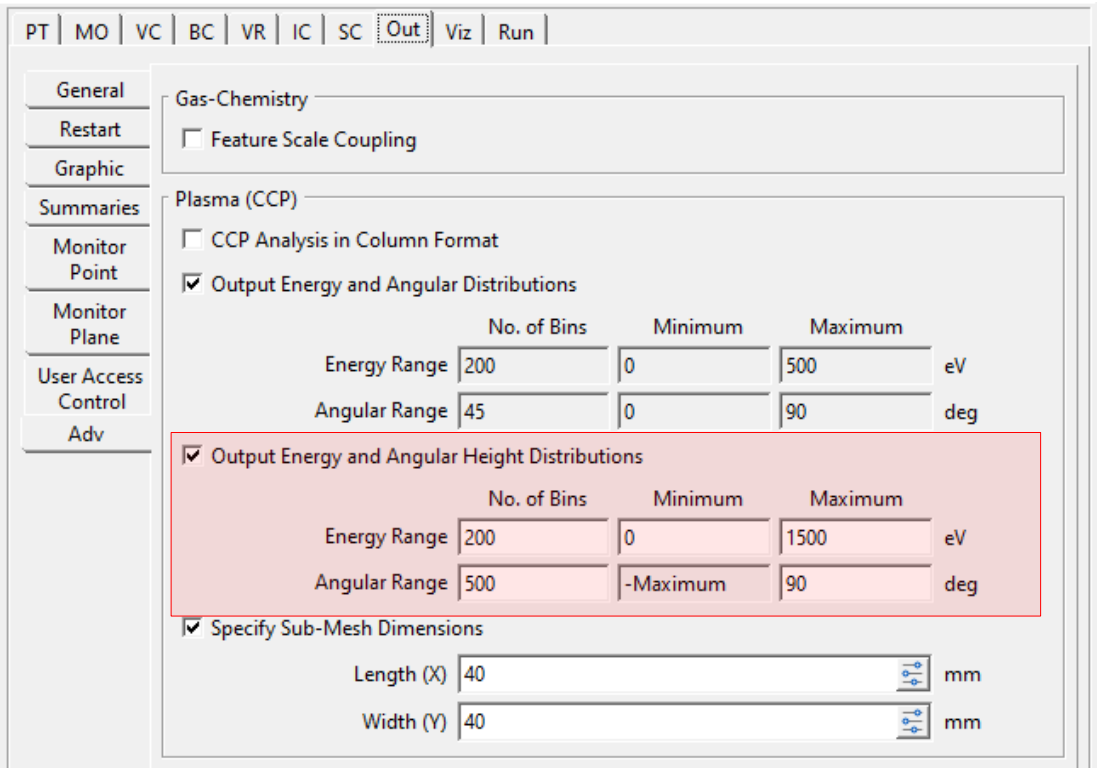
mcplas_elastic_off int 1 1

mcplas_chem2_net_off int 1 1

- Usage
  - » Available through special DTF updates or special solver variables.
  - » There are three options available as described below.
  - » <u>To switch off elastic collisions</u>
    - **mcplas_elastic_off int 1 1**
    - By default, the elastic collisions are on i.e., mcplas_elastic_off int 1 0.
  - » <u>To switch off charge exchange collision</u>
    - **mcplas_charge_exchange_off int 1 1**
    - By default, the charge exchange collisions are on i.e., mcplas_charge_exchange_off int 1 0.
  - » <u>To switch off collision due to Chem2 module</u>
    - **mcplas_chem2_net_off int 1 1**
    - By default, the collisions are on i.e., mcplas_chem2_net_off int 1 0.
  - » These special DTF updates can be used individually or collectively

Energy Bin Control for IEHD and IAHD Visualization

- Enhancement
  - » Users can control the number of bins and range for Ion Energy Height Distribution (IEHD) and Ion Angular Height Distribution (IAHD)
  - » Option activated in Out → Adv → Plasma (CCP)
  - » Helps in improving the resolution for IEHD and IAHD.

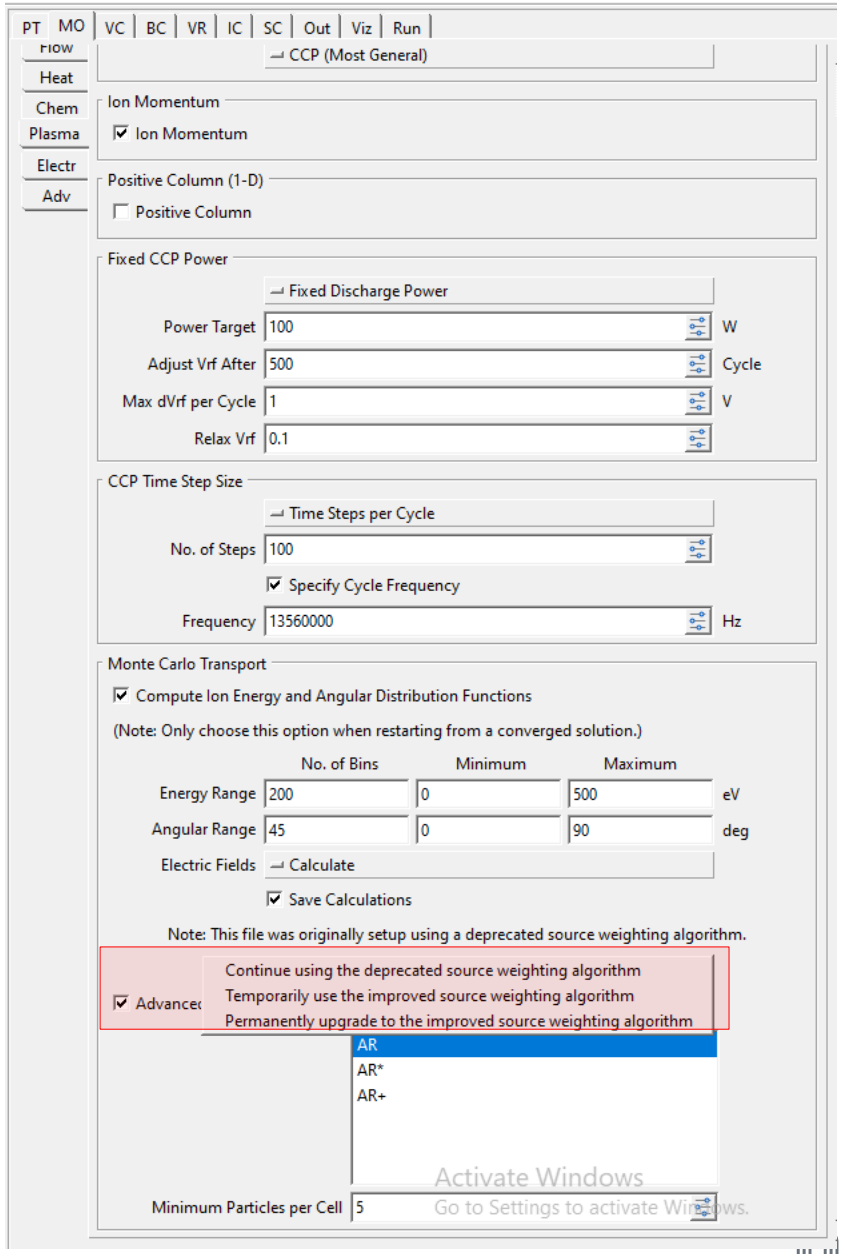


- Usage Guidelines
  - » Minimum, maximum and default values for each of the field are as follows:
    - Energy Range:
      - Energy No. of Bins : minimum = 1, maximum = 5000 and default = 200
      - Energy Minimum : minimum = 0, maximum = 5000 and default = 0
      - Energy Maximum : minimum = 0, maximum = 5000 and default = 1500
    - Angular Range:
      - Angular No. of Bins : minimum = 1, maximum = 1800 and default = 500 (The maximum value of 1800 provides a resolution of 0.1 degree)
      - Angular Minimum: minimum = maximum = default = - Angular Maximum (negative of Angular Maximum)
      - Angular Maximum : minimum = 0, maximum = 90, default = 90

Improved Scheme to Generate Particles in Cells

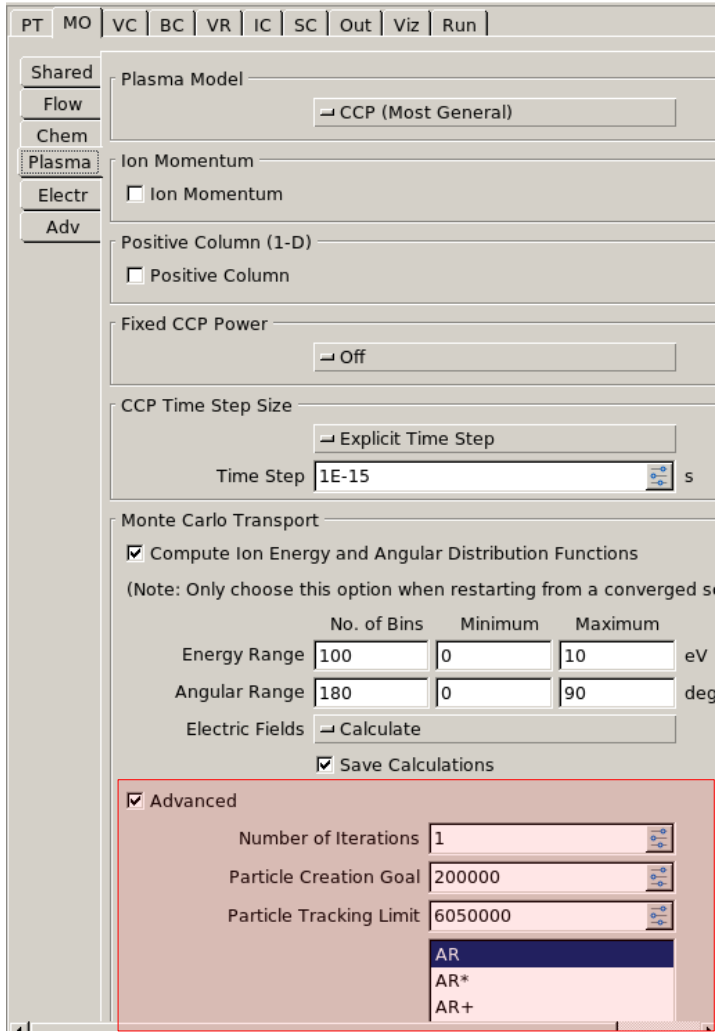
- Improvement
  - » Improvement of weighting function used for calculating the number of pseudo-particles of any species generated from different cells for MC-IEADF calculations
  - » Needed because of dynamic range of source function

- Usage
  - » In the case is setup in ACE GUI 2025.0 or later, the default option is the new weighting function
  - » If a simulation was set-up for MC-IEADF calculation in ACE GUI 2024.0 or earlier, the user will see three options under
    - MO → Plasma → Monte Carlo Transport



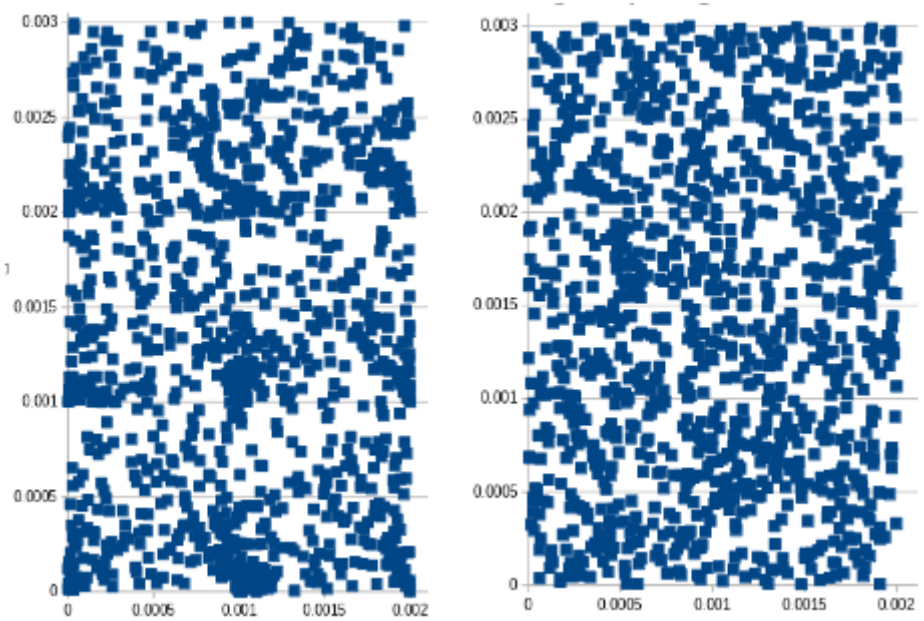
User Specified Number of MC Particles and Iterations

- Improvement
  - » The following DTF update variables to control number of MC particles and iterations can now be directly set through GUI
  - » **Control Iterations:**
    - **niter_mcplas int 1 X**
      - Default value for X now is 10 iterations
  - » **Control number of MC particles:**
    - **num_part_niter_mcplas int 1 Y**
      - Use this number Y as a goal to create MC particles for each iteration, Default value = 6000000
    - **num_part_max_mcplas int 1 Z**
      - During the MC simulation, MC particles can be generated or removed during each iteration.
      - After particles are generated, they will be tracked until they are removed.
      - The total number of particles being tracked cannot be larger than Z, Default value = 6050000



New Particle Identification and Loading Schemes

- Improvement
  - » New particle identification: each particle has its own name id now
  - » New particle loading - positioning: new scheme is able to provide true random position for each particle in a cell
  - » New particle loading - velocity: new scheme is able to provide true maxwellian distribution based on temperature



Old

New

Bug Fixes

- ACE SOLVER
  - » ACE+ Solver STOPS with unknown reason for surface reaction modeling
  - » VOF model crashes for Total Pressure Inlet BC
  - » Profile in Time related
    - Chemistry "profile in Time" specification with AutoDT causes parallel crash
    - Mixture table in the out file
    - OUT file - "profile in Time" mixture values is not printing for the parallel run
    - Profile in Time - Output mixture Profile is incorrect
  - » Plasma MC related
    - Launch of MC particles doesnt match up when using uniform particle distribution
    - inaccurate output variable and title for MC
    - Bug fix for an extra low energy MC pseudo-particle inaccurately created for charge exchange collision
    - Kinetic energy and momentum not conserved after elastic collision

- ACE SOLVER
  - » MC Radiation Output related
    - Finished Tracing: Exceeds 100% for parallel run due to a bug in estimating the number of rays traced on faces/patches
    - Number of Rays Emitted: Very large, even more than the total prescribed rays, for parallel run
    - Inappropriate printing message about ray intersection and ray lost
    - Radiative Heat Fluxes for parallel runs (Net Radiative Heat Imbalance is misleading)
    - 'Could not find material in the database...' printed multiple times
- ACE GUI
  - » Wrong unit conversion from microns to millimeters
  - » GUI crashes when pasting volume reactions in the database manager
  - » Change in behavior of residual plotter
  - » Volume/Surface reactions not dumped in script
  - » GUI allows blank physics input values
  - » Monitor point plot for species mass fraction is not plotted correctly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