Release Notes

ACE+ SUITE

2024.0

Applied Materials Confidential

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Confidentiality Notice

Introduction

This document introduces the V2024.0 release of the ACE+ Suite of applications. It summarizes the new features, enhancements and the list of issues that are corrected since the V2023.0 release.

ACE+ SUITE of Applications

The ACE+ SUITE package includes applications that provide the necessary tools for advanced multiphysics analysis in a virtual prototype environment. The complete list of applications is shown below:

- CFD-GEOM
- CFD-VisCART
- CFD-ACE+
- CFD-FASTRAN
- CFD-TOPO
- SimManager
- CFD-VIEW
- CFD-Toolkit

Supported Platforms

ACE+ SUITE V2024.0 is supported on the following platforms:

Platform	Package Canonical Name
Windows 10 on Intel or AMD (64-bit)	`windows-x64-intel19-msvc142-md`
Linux RedHat Enterprise 7+ on Intel or AMD (64-bit)	`linux-x64-intel19-glibc2.17`
Linux RedHat Enterprise 8+ on Intel or AMD (64-bit)	`linux-x64-intel19-glibc2.28`

> - *ACE+ SUITE is not supported on 32-bit platforms (Windows or Linux).*
> - *If you are not using installers provided by Applied Materials, ensure that you have the right directory structure.*

User Subroutine - Intel FORTRAN Compiler Versions

In the table below, the Applied Materials **ACE+ Version** indicates the version from which a particular Intel FORTRAN Compiler or Visual Studio is supported until replaced with a newer version:

ACE+ Version	Intel Compiler Version (Linux)	Intel Compiler Version (Windows)	Visual Studio Version (Windows)
2023.0	2020.0	2020.0	VS2019

The table below displays the legacy ESI **ACE+ Versions** and supported Intel FORTRAN Compiler or Visual Studio versions and is provided for informational purposes only.

ACE+ Version	Intel Compiler Version (Linux)	Intel Compiler Version (Windows)	Visual Studio Version (Windows)
2013.0	2011.1	2011.1	VS2008
2013.4	2011.1	2011.1	VS2010
2015.0	2015.3	2015.3	VS2010
2017.0	2015.3	2015.3	VS2013
2017.5	2016.4	2016.4	VS2013
2018.5	2016.4	2016.4	VS2015
2021.0	2020.0	2020.0	VS2019

Running Older Versions

Multiple versions of ACE+ SUITE can in general be installed and run in parallel. However, please note that the legacy ESI ACE+ Versions and the Applied Materials ACE+ Suite requires different licenses.

Environment Requirement

If you install V2024.0 software alongside previously installed older version(s), modify your `PATH` environment variable so that the newest `UTILS\bin` directory appears first in your `PATH`.

Then, it is possible to run older versions of the software using the `-runver` **<version>** option from the command prompt or from the MS Windows **Start** > **Run** app.

Example

```
CFD-GEOM -runver 2021.0
```

This command will launch CFD-GEOM software V2021.0.

To use -runver option with both the legacy ESI ACE+ versions and Applied Materials ACE+ Suite, it is recommended that the users install both the software in the same directory. This enables the environment variables **ESI_HOME** (used by the legacy version) and **ACE_SUITE_HOME** (used by the new versions) to be the same.

License Requirement

You will need a V2024.0 or later license to run V2024.0 applications.

Flexnet V11.19.1 (provided in this package or downloadable from the Applied Materials Portal) should be used for the V2023.0 and later applications to work.

- Install the FNP Licensing Service (install_FNP) provided in the toolkit.
- Run the getLmHostIds program (from a terminal) to get the host information needed for license generation.
- Use the lmadmin program to install and administer the license. Refer to the README.txt file and the fnp_LicAdmin.pdf manual within the Flexnet toolkit for detailed instructions.

Installation

This section summarizes the main steps to install ACE+ SUITE.

Installing ACE+ SUITE on Windows

1. Extract the **ACE+Suite_V2024.0_Windows-x64.zip** archive to a temporary directory.
2. Click **setup.exe** and follow on-screen instructions.

The installer will install the necessary packages and set up the environment variables (ACE_SUITE_HOME and PATH).

Installing ACE+ SUITE on Linux

1. Extract the **ACE+Suite_V2024.0_Linux-x64-glibc2.17.tar.gz** (for RHEL 7) or **ACE+Suite_V2024.0_Linux-x64-glibc2.28.tar.gz** (for RHEL 8) archive to a temporary directory.
2. From within the extracted directory, run **install.com** and follow on-screen instructions to complete installation.
3. Login as the end user and run **configure_user_account.sh** to setup the necessary environment variables (ACE_SUITE_HOME and PATH).

Manually Setting Up Environment Variables

1. Set the ACE_SUITE_HOME environment variable. This defines the directory where the software is installed:
   - Windows:

     ACE_SUITE_HOME = C:\Program Files\Applied_Materials

   - Linux – BASH:

     export ACE_SUITE_HOME=/usr/local/Applied_Materials

   - Linux – CSH:

     setenv ACE_SUITE_HOME /usr/local/Applied_Materials

2. Set the `PATH` environment variables. They should reflect the new path to `UTILS/bin`.
   - Windows :
     `Variable Name:` **`PATH`**
     `Value:` **`%ACE_SUITE_HOME%\ACE+Suite\2024.0\UTILS\bin`**
   - Linux – BASH :
     `Variable Name:` **`PATH`**
     `Value:` **`$ACE_SUITE_HOME/ACE+Suite/2024.0/UTILS/bin`**
     `Command:` **`export PATH=$ACE_SUITE_HOME/ACE+Suite/2024.0/UTILS/bin:$PATH`**
   - Linux – CSH:
     `Variable Name:` **`PATH`**
     `Value:` **`$ACE_SUITE_HOME/ACE+Suite/2024.0/UTILS/bin`**
     `Command:` **`setenv PATH $ACE_SUITE_HOME/ACE+Suite/2024.0/UTILS/bin:$PATH`**

New Features and Enhancements

This chapter describes the new features and improvements of ACE+ SUITE V2024.0 release.

CFD-GEOM

CFD-GEOM V2024.0 includes the following new features and enhancements. Please refer to the *ACE+ SUITE 2024.0 CFD-GEOM User's Guide* for further details.

Enhanced Performance for Rendering Large and Complex Models

V2024.0 CFD-GEOM significantly improves the speed and efficiency of graphical rendering for large and complex models, ensuring a smoother and more responsive experience. An alternate texture-based method has been introduced to draw the lasso box and avoid graphical artifacts.

The latest release also introduces a major performance improvement in the performance of transformation operators, including translate, rotate, scale and scale all. Users will now experience faster and more accurate previews, while also benefiting from reduced memory usage.

A new, optional selection mode, specifically for faster selections in large models, has been introduced. Currently, CFD-GEOM has one selection mode that is software-based method and selects entities based on mouse click or lasso. With the new tool, objects obscured by closer objects will not be selected. Thus, a single click will only return the closest object and nothing else while a lasso selection will only select the non-obscured objects. A new button is added to the main toolbar to switch selection modes. This setting will be retained in the global settings and will be set/unset on a new invocation of CFD-GEOM.

Figure 5-1: Fast Selection Mode

CFD-GEOM supports up to 10 quick views with custom names. These views are saved in the GGD file and can be recalled using short cuts. To create and save a view, use **`Ctrl + Alt + (0-9)`**. You can manage the names by right clicking in the graphical viewer and select **`Quick Views > Manage Names`**. To recall and activate a view, use **`Ctrl + (0-9)`**.

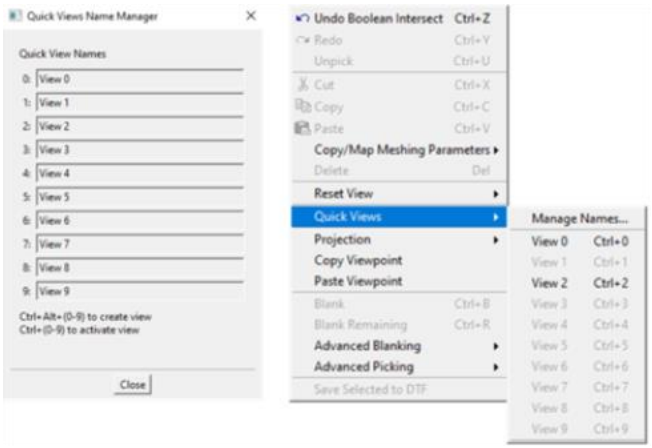

Figure 5-2: Save and restore Quick views with custom names

The current model tree displays each entity in their own folders. However, the ordering is based on the order of creation. Now, CFD-GEOM will order the items in each folder alphabetically according to assigned names, thus, making it easier to locate items. In addition, meshed solids are now highlighted through a different icon.

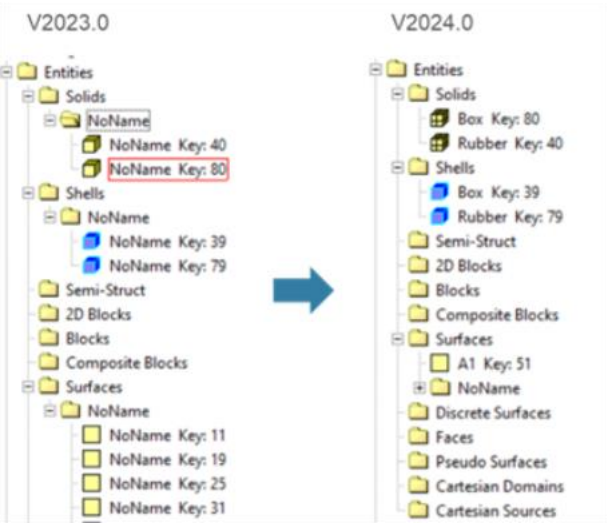

Figure 5-3: Model tree enhancements

Selective Part Import Capability

CFD-GEOM supports the import of CAD models in different formats. In current versions, the whole model is imported. However, there are situations when it is necessary to import only a subset of the parts in the CAD model. This may be necessitated by the need to focus on repairing a component or replacing a part in a design study.

The file import dialog has been updated with a new **`Allow Selective Import`** option. Upon enabling selective import, a dual graphics window interface is presented. The left side displays all parts of the CAD model. Users can select desired parts on the left side and then move it to the right side for importing into CFD-GEOM.

Accompanying this new option is the ability to generate thumbnails for various parts of the CAD model. This visual aid can enhance the selection process for some models.

Beside facilitating selective importing, the dual viewer setup also serves as a tool to interrogate and understand a model before importing into CFD-GEOM.

The selective import feature is also available while replacing parts in CFD-GEOM.

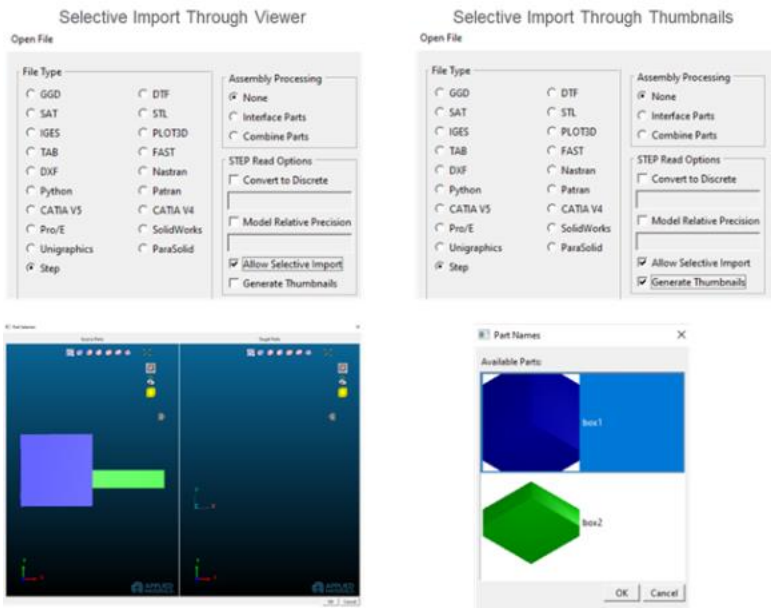

Figure 5-4: Selective import of parts

New Solid Inversion Tool

The Invert Model tool in CFD-GEOM allows users to extract fluid domains from a 3D CAD model. This tool works on the entire model and not just a subset. For large models, this could cause the creation of hundreds of unneeded domains. Other limitations include not working with non-planar holes and not supporting undo/redo of the inversion operation. A new method is added to this tool which removes the above-mentioned limitations.

To invoke this tool, select the **`Selected Domains`** Inversion Type. Then, select a subset of available unstructured domains. Immediately, all possible capping surfaces are displayed, and all remaining surfaces are hidden. Select relevant bounding surfaces which reveals holes formed by the bounding surfaces and apply to perform the inversion operation.

The new method works with non-planar surfaces and supports undo/redo operations.

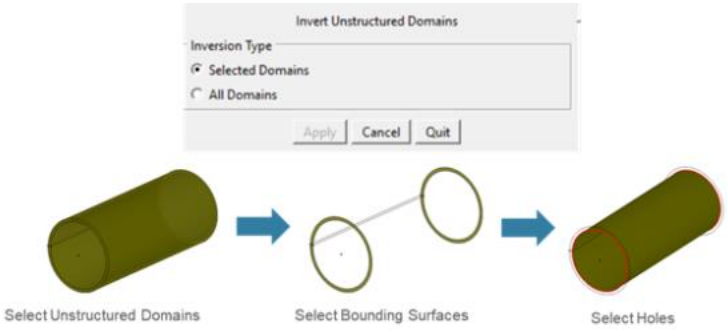

Figure 5-5: Unstructured domain inversion tool

Improved Cut Section Tool

A new cut section tool was introduced in V2023.0. This tool has been improved in V2024.0. Users can expect faster performance for larger models. Along with enhanced graphics, display of outlines of the cut section and automatic clipping of the region away from the cut plane is enabled. Interactive distance measurement on the cut sections is now possible on the cut section or the model. This tool now serves two purposes, the first being to create arbitrary planar cut sections in solids and secondly for visualization to interrogate models.

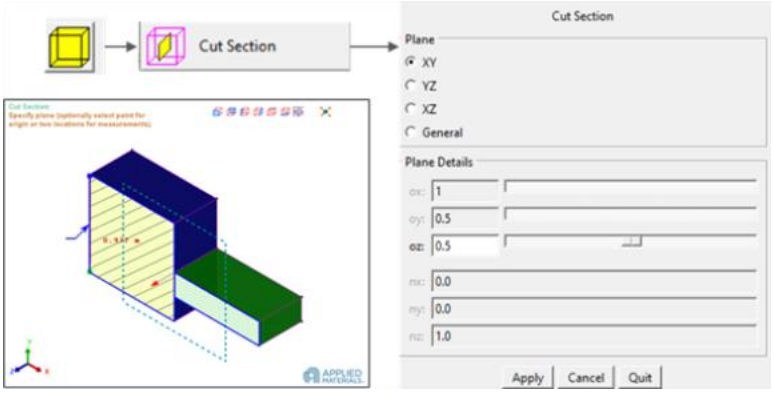

Figure 5-6: Cut section tool

Meshing Improvements

An expansion factor for Advancing Front (AF) Surface meshing has been added to allow the user to obtain a mesh with fewer interior elements.

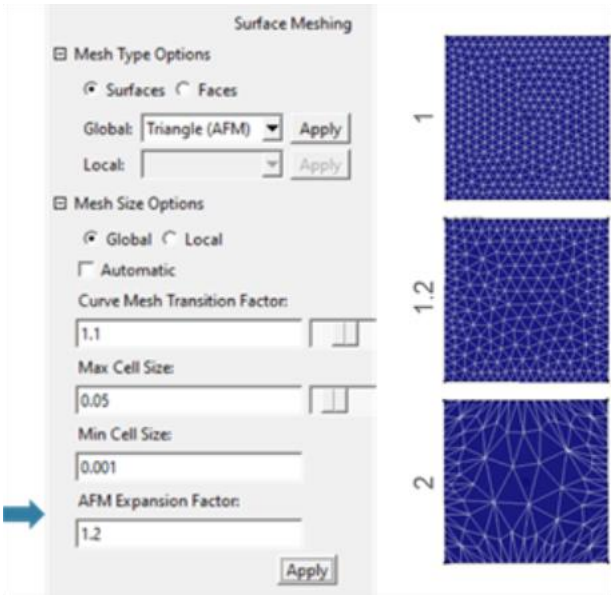

Figure 5-7: Advancing Front surface meshing tool

The following additional performance improvements are available with the Advancing Front (AF) Surface meshing option in CFD-GEOM.

1. Improved interior curvature resolution.
2. Improved mesh element sizes when using Octree background for sizing.
3. Advancing Front Tetrahedral meshing performance improvements to generate 60K to 300K more elements per minute.

Additional Robustness and Performance Improvements

A revised distance measurement tool is now available to interactively interrogate feature sizes with improved performance for minimum distance tool, especially for large models.

A revised 3D mesh quality tool for Unstructured Domains, Semi-structured domains, and 3D Structured blocks is now available. Entities which violate a given quality criteria will now be highlighted and pressing Ctrl + r will hide all other visible entities.

A bug fix for reading large python scripts significantly reduces time for models with large number of geometric entities.

Improved handling of spherical and conical surfaces to eliminate trimming failures.

File import times for large CAD models is faster and robust. Users no longer need to iteratively change parameters to obtain the cleanest import for most models.

CFD-VisCART

CFD-VisCART V2024.0 includes the following new features and enhancements. Please refer to the *ACE+ SUITE 2024.0 CFD-VisCART User's Guide* for further details.

Selective Part Import Capability

CFD-VisCART supports the import of CAD models in different formats. In current versions, the whole model is imported. However, there are situations when it is necessary to import only a subset of the parts in the CAD model. This may be necessitated by the need to focus on repairing a component or replacing a part in a design study.

The file import dialog is updated with a new Partial importing by selecting parts option. Upon enabling selective import, a dual graphics window interface is presented. The left side displays all parts of the CAD model. Users can select desired parts on the left side and then move it to the right side for importing into CFD-VisCART.

Beside facilitating selective importing, the dual viewer setup also serves as a tool to interrogate and understand a model before importing into CFD-VisCART.

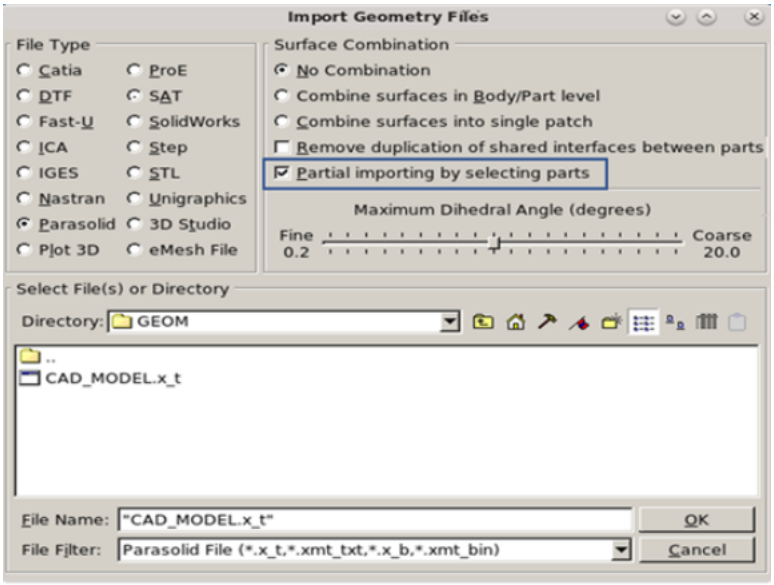

Figure 5-8: Selective import of parts

Save and Restore View Quickly

CFD-VisCART now allows to save and restore up to 10 views of a model. These views can have unique names and will be stored in the .VGD file when saved. These options can be invoked

from **View > Save view or View > Switch view**. The same options can also be accessed using shortcuts **(CTRL+ALT+(0-9)** to save view and **CTRL+(0-9)** to restore view).

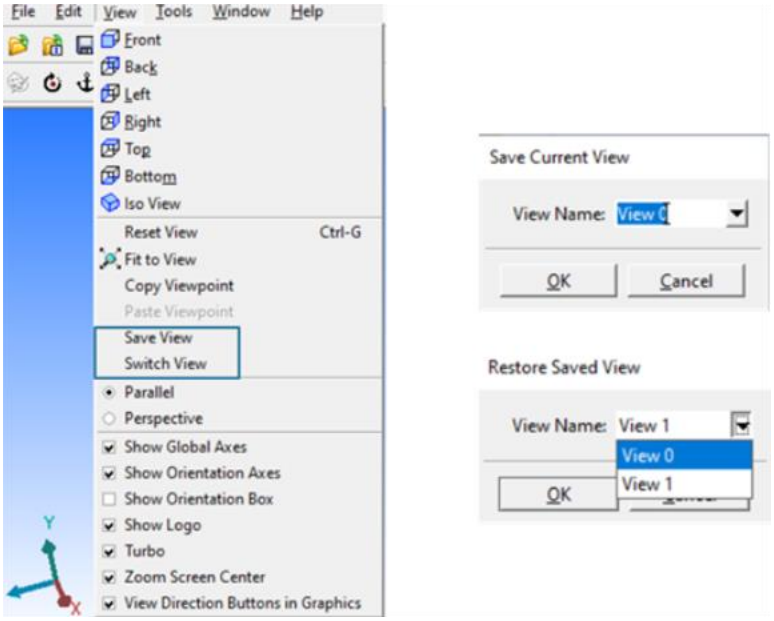

Figure 5-9: Save and restore view

Enhancements Related to Solids/Groups

1. Groups/Solids can now be sorted in ascending, descending or the original (default) order.
2. When a surface is selected in GUI, the Group/Solid to which it belongs, will be highlighted in the explorer. If the surface belongs to both Group and Solid, then Group takes precedence and will be highlighted.
3. 3. When a surface is selected in GUI, Group Blanking/Solid Blanking options **(Hide, Show, Hide Others, and Inverse Visibility**) can be invoked from the right-click menu. **Hide, Show and Hide Others** work as the name suggests. **Inverse Visibility** will inverse the groups/solids displayed in GUI.
4. When cursor is hovered over Group(s) or Solid(s) panel, the status bar shows the count of Groups and Solids in the model.
5. 5. While grouping/regrouping surfaces, the option **Remove selected item(s) from old group** is introduced to prevent duplicates.

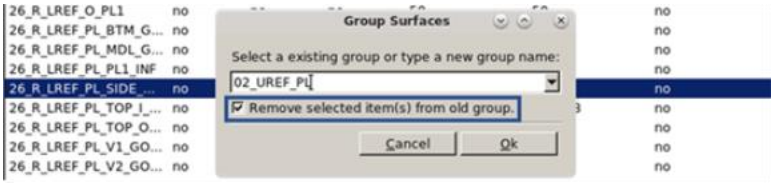

Figure 5-10: Prevent duplicates while grouping

6. The explorer search tool has been enhanced to restrict search for surfaces to specified solids in the model. A new operator keyword “solid:” can be used to restrict searches to specific solids in the model. For example, solid:solid_1 name:surface_1 will look for objects with name surface_1 within the solid “solid_1”.

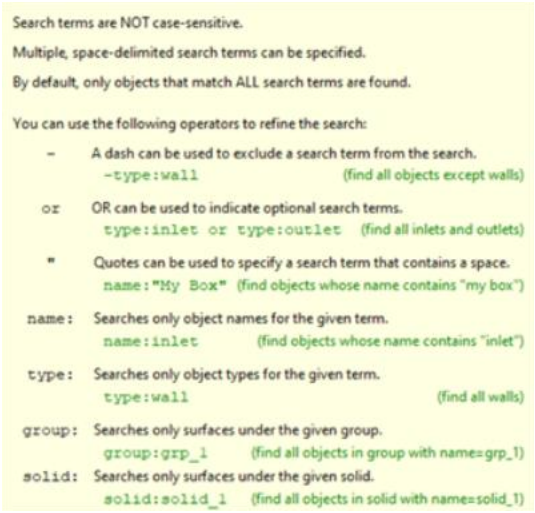

Figure 5-11: Enhanced search tool – additional operator keywords

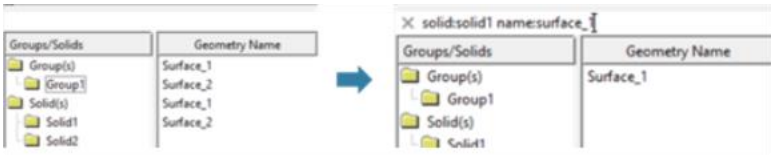

Figure 5-12: Enhanced search tool - usage

Cylindrical Source Enhancements

The cylindrical source detection capability in CFD-VisCART allows users to identify and apply mesh refinement sources on multiple similar cylindrical components such as those in showerhead holes. This capability has been enhanced to handle non-flat (slanted) top or bottom surfaces. In addition, once cylindrical sources are detected, the height of the sources

can be extended downstream beyond the cylinder to have smooth mesh transition to capture important flow features. The direction of the extension can be reversed using the "Reverse Direction" option. All similar cylindrical sources will be oriented in the same direction of the parent cylindrical source.

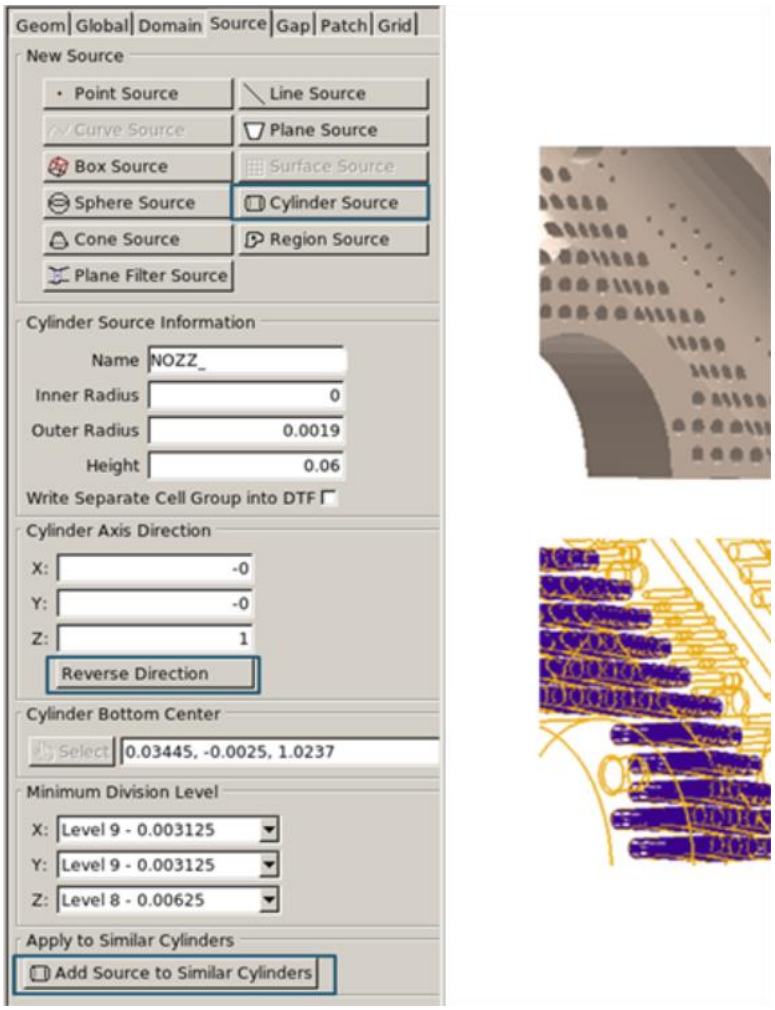

Figure 5-13: Enhanced cylinder source for mesh refinement

Export a Subset of Domains to DTF

CFD-VisCART, in previous versions, exported all meshed domains to DTF and users did not have control over which ones to export. This is useful in large models where a user may be interested in testing a subset of the model. Users can now right-click on selected domains and use the option, **`Save Selected Domain Mesh to DTF`**, and export a subset of meshed domains to DTF.

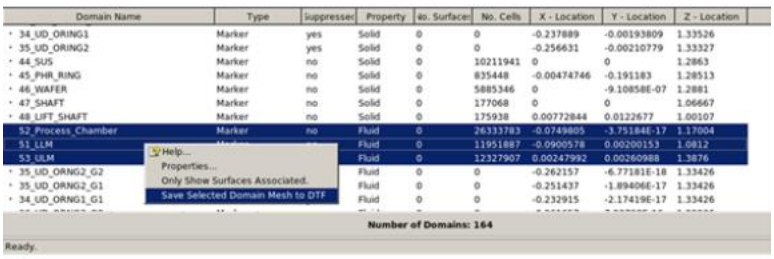

Figure 5-14: Export subset of domains to DTF

Additional Performance and Robustness Improvements

1. Distance measurement has been enhanced to support measurement between a point and a surface (in addition to the previously supported options to measure distance between two points or a point and a line).
2. Renaming of multiple patches is supported now. When multiple patches are selected, CFD-VisCART will auto-generate and add a number to the given new patch name as a suffix.

Figure 5-15: Rename multiple patches

3. CFD-VisCART now allows to modify patches even after meshing. This enables users to combine/split patches before writing to the DTF file.
4. Part names are now read and preserved for Parasolid Import.

CFD-ACE+

CFD-ACE+ V2024.0 includes the following new features and enhancements.

Please refer to the *ACE+ SUITE 2024.0 CFD-ACE+ User's Guide* for further details.

Improvements to Parametric Study Capability

CFD-ACE+ supports the use of parameters on most inputs. These parameters can then be used as part of a parametric study to evaluate the effects of varying such parameters within a given range of values. In recent releases, this capability has been extended to some of the inputs in the database, particularly, the ability to vary mixture flow rates (SLM or SCCM). In this release, this has been extended to volume and surface reaction parameters - Pre-exponential Factor (Ap), Activation Temperature (Ea/R), Temperature Exponent (n), Pressure Exponent (m) and Sticking Coefficient (Sc).

To set these inputs as parameters, select **Tools > Parameters and Expressions > Parametric Reactions**. A list of volume and surface reactions in the model will be displayed. For each reaction, users can set any of the available input as a parameter. Note that Sticking Coefficient is applicable only for surface reactions and the pressure exponent is not available as a parameter for surface reactions.

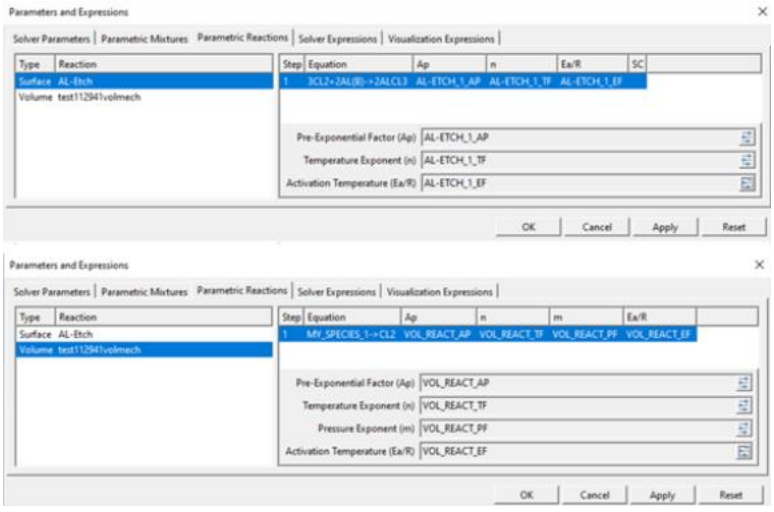

Figure 5-16: Parametric reactions

In previous versions, cases in a parametric study will run sequentially and post-processed for any Visualization Expressions setup in the model (done through the Viz tab) as soons as the run is complete. From this release, parametric studies can run multiple cases

simultaneously. The maximum number of concurrent runs can be controlled from `Edit > Preferences > Parametric Studies > Maximum number of concurrent solver runs`.

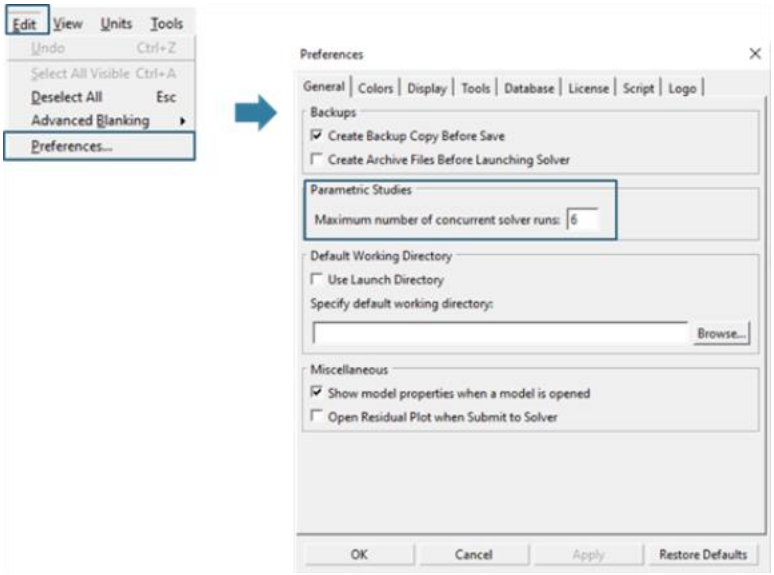

Figure 5-17: Concurrent runs for parametric studies

Each concurrent run requires an additional solver license. Each case can also be run in parallel mode using mpi and / or threading and would use necessary licenses.

Reinstatement of Structural Dynamics Module

Due to certain licensing issues, the structural dynamics module was disabled in the 2023.0 version. This limitation has been removed. Users can avail the use of this module again from this release.

In previous versions, all solid domains involved in stress simulations must be part of a single process in a parallel run (other modules may be run in multiple processes). This limitation has been removed and the module is now supported in parallel.

Certain features of the module are still unavailable (modal analysis) and will become available in future releases. If solid shell elements have multiple elements across the thickness and these elements are on different processors, parallel mode is not supported.

Improvements to Heat Transfer Modeling

The Thin Wall Boundary Condition simulates physical features such as baffles, plates, and heat resistances whose thickness is so thin as to be essentially ignorable from a grid

generation perspective, but not from a momentum, heat transfer, and/or scalar transport standpoint. In recent versions, CFD-ACE+ had added support for multi-layer thin walls and solid borders while allowing variations in thin wall thickness and account for temperature dependent variations in thermal conductivity. However, the underlying formulation was a steady-state approximation even in transient simulations. In this release, this limitation has been removed. Users will additionally input Specific Heat and Density of the material involved.

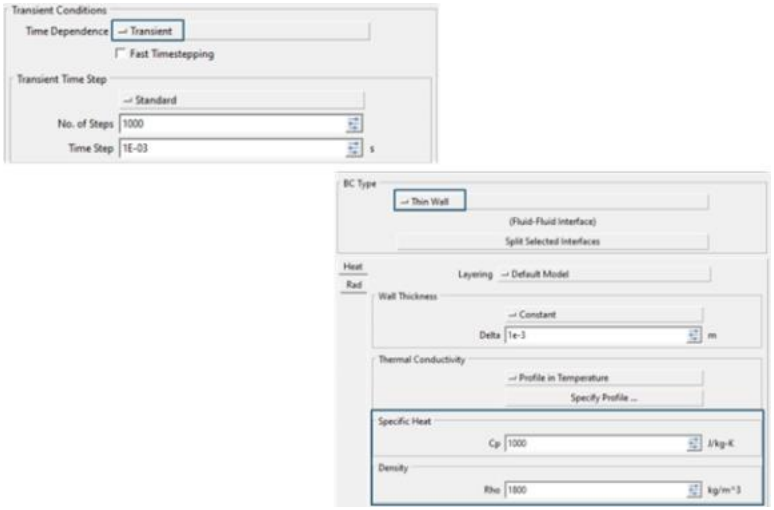

Figure 5-18: Thin wall specification for transient runs

In CFD-ACE+ Thin Wall Boundary Condition, a higher fidelity contact resistance calculation may be made with the addition of thermal gap modeling. This model is used to calculate the heat transfer between solid bodies separated by a gap. The thermal gap model accounts for gaseous conduction within the gap, the effects of direct-contact conduction (solid-solid conduction), and radiation across the gap. In previous versions, users had to specify one emissivity value for the gap model. In situations, where there are materials with different emissivities on each side of the thin wall, users had to calculate an effective emissivity for the thermal gap. In this version, users will have the option to specify the emissivities of each side directly in GUI.

If users wish to specify the emissivities on either side of the thin wall directly, uncheck the **`Use the same emissivity for both sides`** check box, and specify the values for the near side and far side emissivities. The near side is represented by a yellow arrow and the far side is represented by a red arrow. Use the **`Reverse Sides`** check box to switch directions (also reflected by the arrows).

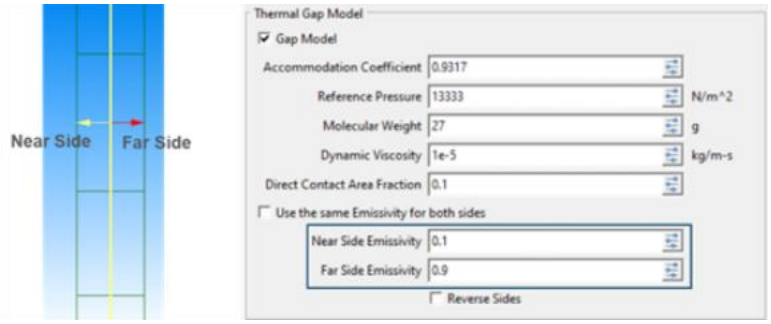

Figure 5-19: Thermal gap model – emissivity specifications

Spectral properties calculated during a Monte Carlo radiation simulation can be written to a file by checking Spectral Properties check box in **`Out > Adv`**. This issue has been corrected and the calculated Planck-averaged transmittance data is correctly written to the MC file.

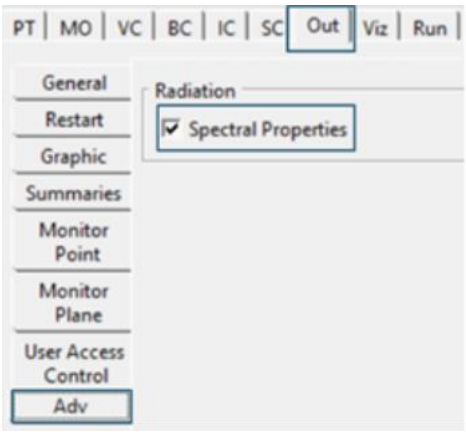

Figure 5-20: Writing calculated spectral properties to an external file

When **`Out > Summaries > Energy Balance Summary > Monitor Energy Imbalance`** is switched on, energy imbalance data is written to the *_IQ.MON file at every iteration. However, a previous bug prevented the inclusion of volumetric heat sources at every iteration. Instead, it was added only when a DTF was written out. This issue has been corrected to include volumetric heat sources at each iteration. Note that this issue was restricted to the *_IQ.MON file only and does not affect the simulation results itself.

Improvements to Chemistry Modeling

Thermo diffusion, also known as Soret Diffusion, accounts for diffusion that arise due to temperature gradients. Corrections and improvements have been made to the temperature gradient calculations and the Soret source term, potentially improving accuracy and convergence.

In Finite-Rate (Species Approach in Gas Phase) - Multistep reaction with Third Body (M) and pressure dependency, users have the option of providing parameters for pressure fall-off reactions. In CFD-ACE+, Unimolecular/Recombination and Chemically Activated reactions are allowed with different blending functions. A defect prevented the parameters from being read for Unimolecular/Recombination reactions. This issue has been corrected along with minor improvements to the output.

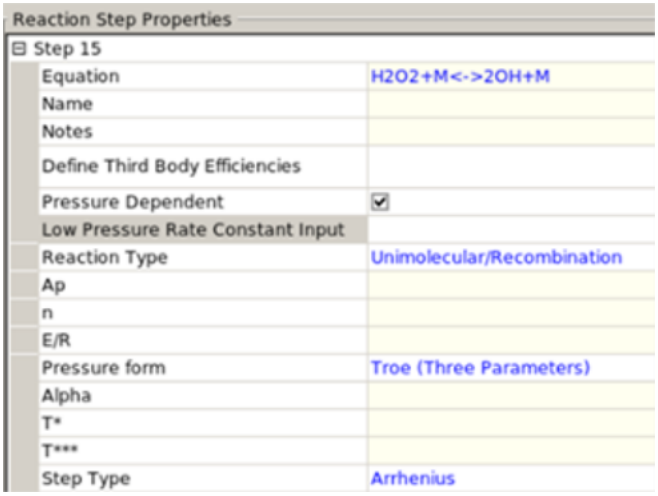

Figure 5-21: Pressure fall-off reactions specifications

Users can now monitor mole fractions through the monitor points facility of CFD-ACE+. Previously, it was restricted to Species Mass Fractions (Gas Phase) or Species Concentration (Liquid Phase). This can be used as an additional way of ensuring that a case has converged.

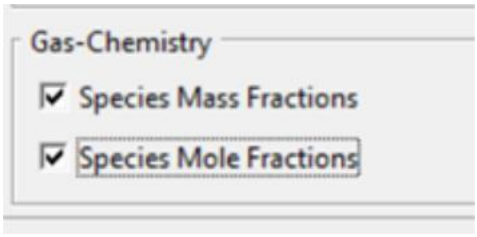

Figure 5-22: Monitor Species Mole Fractions

For Species Mass Fraction monitor points, users may also notice that values less than 1E-30 are now written as 0 to address certain format / plotting issues.

In some cases, with Species Mass Fractions monitor points, the solver may crash during a parallel run in previous versions. These issues have also been addressed.

The **`Profile in Time`** for mixture specification allows users to easily input ALD type inlet boundary conditions. Users can input the different steps of an ALD cycle easily and specify the number of cycles to simulate. Several corrections and improvements have been made to

ensure that the specified input table (time steps and mixture flow rates) is honored. Note that at this time, input to the table is the ratio of a mixture as compared to its value specified in the database. In general, the solver linearly interpolates between the two rows in the table within which the current simulation time falls and an exact timestep size of zero is currently not possible. Therefore, a small timestep size is needed even for a step change in gas mixtures. For cycles involving such step changes, it is recommended to use Auto Time Step over the Standard Time Step scheme because of the flexibility it provides to adjust timestep sizes and keep it closer to the actual inputs.

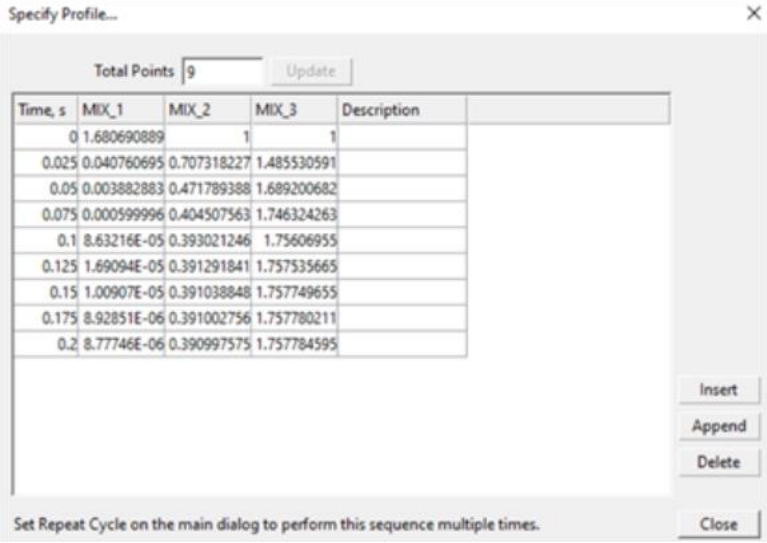

Figure 5-23: Profile in time for mixtures

In the table shown above, for example, the first row should be interpreted as:

1.680690889 * SLM (or) SCCM specified in the database for MIX_1 (which is Mixture_1_BDA) +

1.0 * SLM (or) SCCM specified in the database for MIX_2 (which is Mixture_2_AR) +

1.0 * SLM (or) SCCM specified in the database for MIX_3 (which is Mixture_3_O2)

The solver calculated values at each time step is also printed to the .OUT file.

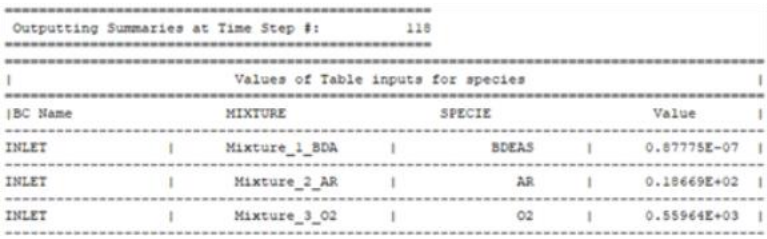

Figure 5-24: Output of calculated inputs for species

Improvements to Multiphase Modeling

CFD-ACE+ Two Fluid module offers two solution approaches for handling phase change problems, the General method, and the Enthalpy method. For the Enthalpy method, Phase change properties of Saturation temperature and Latent Heat of Vaporization are provided in **`MO > Fluid2`** and these properties remain the same for all applicable two-fluid volume conditions. However, in some scenarios, the ability to specify different phase change properties for different volumes can be useful. For example,

- Different phase change properties can be used in problems where the volumes are physically separated from each other and have distinct phase-change behaviors. Examples include microchannel heat exchangers having disconnected hot-fluid paths and cold-fluid paths. It is expected that the disconnected paths may have different gas-liquid properties and phase change properties.
- The ability to provide different phase change properties can also be useful to turn OFF the Enthalpy-based phase-change in a specific volume by setting the Saturation Temperature and Latent Heat of Vaporization to extreme values. This could aid in convergence of the overall problem when no phase-change is occurring in certain volumes.

Enthalpy method in CFD-ACE+ V2024.0 now allows the user to specify different Phase Change properties for each volume condition.

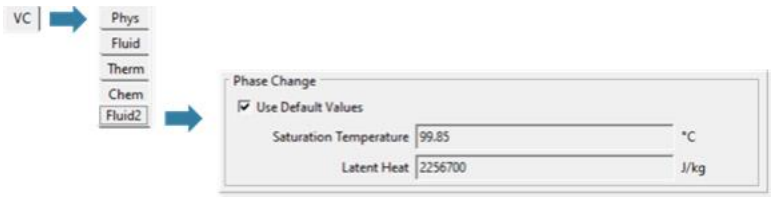

Figure 5-25: VC-by-VC specification of phase change properties

The Spray Module tracks a discrete phase (liquid droplets, solid particles, or bubbles) through the calculation domain. An incomplete time integration for the drops when crossiing over across process boundaries in parallel simulations, caused incorrect trajectory calculations for some parcels in the simulation. This issue has been corrected and the correct parcel locations are calculated even after crossing processor boundaries.

Improvements to Plasma Modeling

Energy and angular distribution (EADF) files can be written out by CFD-ACE+ feature scale output for each ion species, if a sheath model is activated in a plasma reactor scale

simulation. This capability has been extended to CCP simulations. To enable writing the combined EADF file.

1. Restart from a converged CCP simulation
2. Enable Monte Carlo Transport to Compute IEADFs (**`MO > Plasma > Monte Carlo Transport`**)

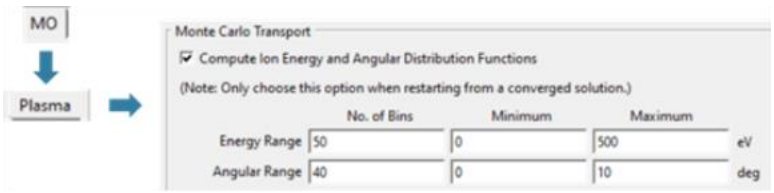

Figure 5-26: Enabling Monte Carlo Transport

3. Set Number of bins, Energy range and Angular range
4. Select MC Output points (**`BC > Output > Plasma > Monte Carlo Transport > Select locations for IEADF Computation`**)

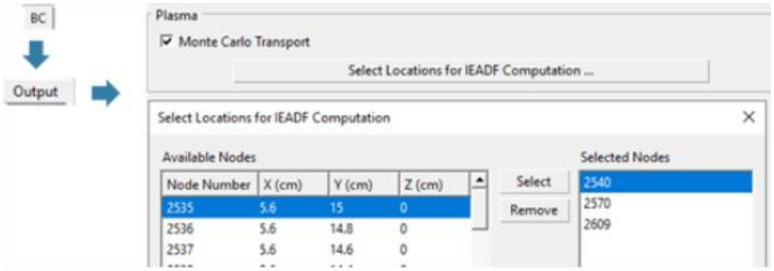

Figure 5-27: Node selection for MC transport

In addition to the EADF files, ion flux information is also needed by CFD-TOPO solver. This is enabled from **Out > Adv > Feature Scale Coupling**. Here, users can choose to manually specify a set of points (**User Input), Read from a file or Use Monte Carlo Transport Locations**. The later would use the same points as specified in **BC > Output > Plasma > Monte Carlo Transport > Select locations for IEADF Computation**.

Figure 5-28: Use MC transport location for feature scale coupling

Users can now optionally save the Electric Field calculated during a Monte Carlo Transport computation for IEADFs. During subsequent MC runs, users can use the saved Electric Field and run the IEADF calculations.

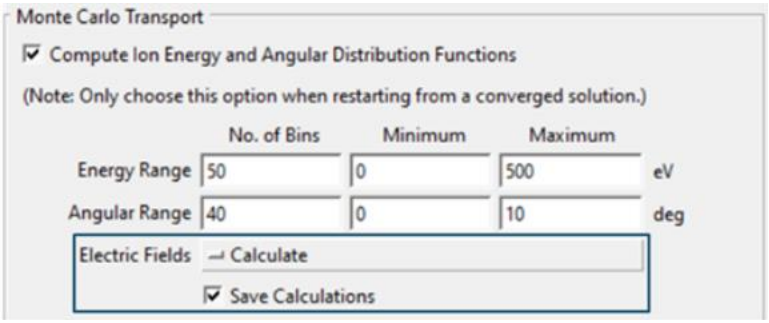

Figure 5-29: Save electric fields or reuse save electric fields in MC transport

MC simulations use a sub-mesh around the chosen output points to minimize computational cost. In some circumstances, this sub-mesh may need to be extended to ensure good statistics. Users can now change this sub-mesh directly from the **GUI Out > Adv > Plasma > Specify Sub-Mesh Dimensions** and enter the X and Y dimensions.

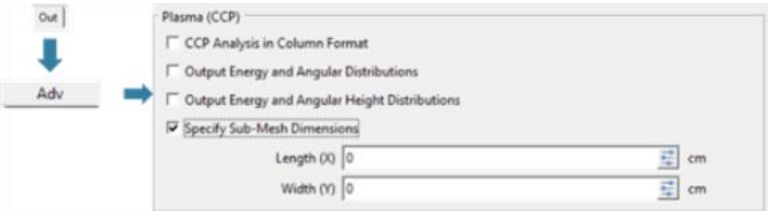

Figure 5-30: Sub-Mesh specification for MC transport

CFD-TOPO

CFD-TOPO V2024.0 includes the following new features and enhancements.

Please refer to the ACE+ SUITE 2024.0 CFD-ACE+ User's Guide for further details.

Improvements to Multi-layer Multi-material Deposition

CFD-TOPO predicts how the shapes of objects will change due to the combined effects of chemical species transport and surface reaction at gas-solid interfaces. CFD-TOPO is applicable for predicting the effects of depositing into, or etching from, relatively small topographical features by gas-phase processes such as chemical vapor deposition or plasma-enhanced etching.

CFD-TOPO can address the deposition and/or etching of multiple materials. However, the data structure implicitly assumes a 1:1 matching between level set functions and solid materials. If the same material is deposited a second time, users may have to manually restart using results from a previous step, which is not convenient. In this release, CFD-TOPO data structure has been upgraded to allow multiple level set functions for a given solid material within the model domain. Now, users can simulate processes in which multiple layers of varying materials are deposited in a feature, including possibly repeating layers of one or more materials and/or intermediate etch steps.

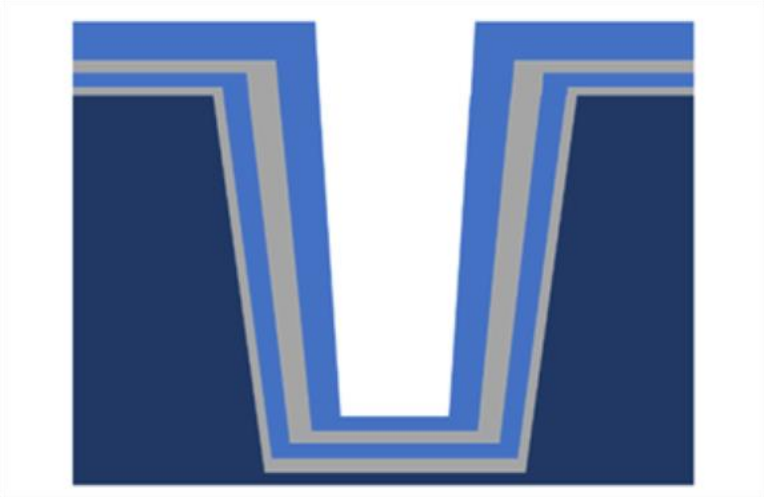

Figure 5-31: Multilayer deposition and etch process

Support for Parallel

Modern high aspect ratio features, or multiple material deposition and etching simulations impose several challenges for simulations. There is an increased necessity for rapid turnaround time in such simulations to enable large parametric evaluations. CFD-TOPO solver has been upgraded to support parallelization through threading. The maximum number of threads to be used can be set from **Edit > Preferences > General > Performance > Maximum number of solver threads**.

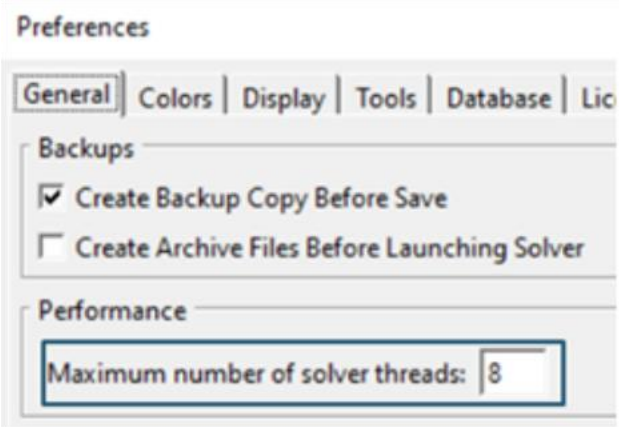

Figure 5-32: Number of threads for TOPO solver

Improvements to Scripting and Parametric Studies

Though a preliminary scripting capability was present in previous versions of CFD-TOPO, it did not support certain section of the application (e.g. RC tab). These limitations have been addressed and CFD-TOPO supports scripting for all features.

Similar to CFD-ACE+, CFD-TOPO now supports the ability to do parametric studies. Users can mark most input fields as a parameter and include it in a parametric study. This also extends to certain database parameters such as Pre-exponential Factor (Ap), Activation Temperature (Ea/R), Temperature Exponent (n) and Sticking Coefficient (Sc).

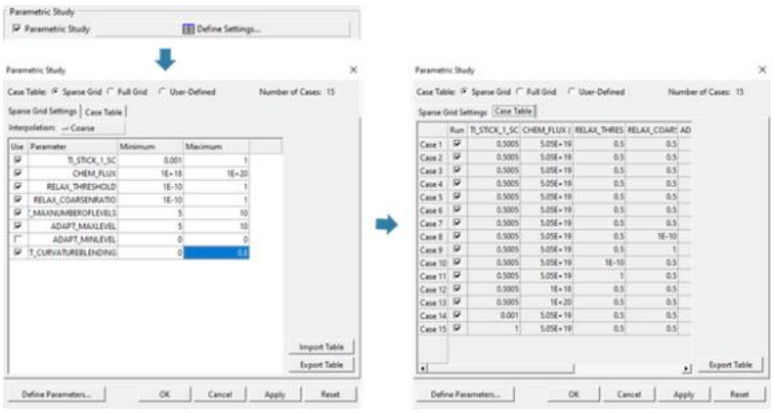

Figure 5-33: Parametric study setup in CFD-TOPO

During a parametric study, multiple cases can be run concurrently. The maximum number of concurrent jobs can be set in **Edit > Preferences > General > Parametric Studies > Maximum number of concurrent solver runs**.

Figure 5-34: Concurrent runs for parametric studies

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