Isothermal Non-reacting Gasifier
Part 1: Presentation

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Training Objectives

Introduction to complex Barracuda model (coal gasifier)

General modeling & simulation principles

- Why are we running a simulation?
- What do we want to learn?
- What level of detail is required?
- What amount of time needs to be simulated?
- What simplifications can be made?

Strategies for getting useful answers quickly

- Run coarse models before detailed models

Barracuda Training Coal Gasifier

The purpose of this model is to provide a realistic example of the types of systems that people typically model using Barracuda.

Complex geometry

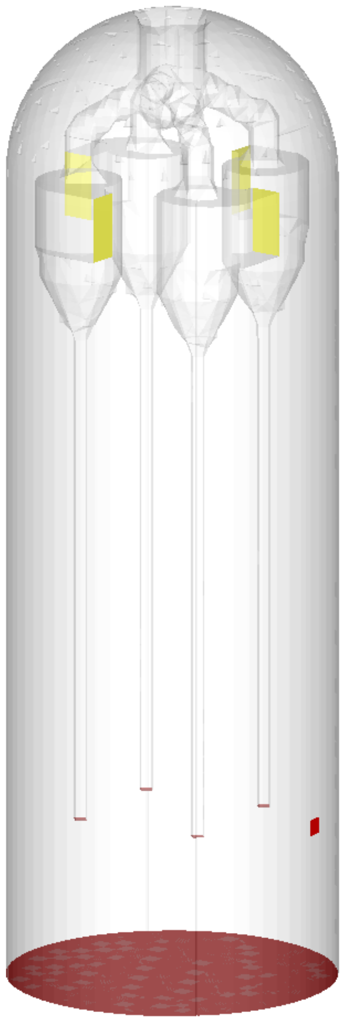
- Internal cyclones
- Internal heating coils
- Internal gas sparger

Complex operating conditions

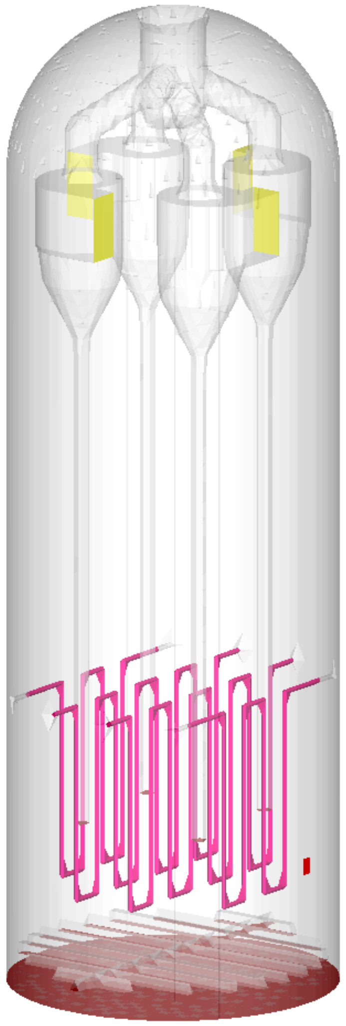
- Multiple gas inlets and outlets
- Multiple particle inlets and outlets
- Chemistry and thermal are important

For training, we will define 2 models:

- Simplified, isothermal, non-reacting case
- More detailed, chemistry + thermal case



Simplified geometry, isothermal



Complex geometry, thermal + chemistry

Questions to Ask About Every Simulation You Run

Why are we running a simulation?

- Designing a new process and want to predict performance through simulations.
- Trouble-shooting a problem with an existing process and want to understand the cause of the problem better.

What do we want to learn from the simulation?

- Answers to this question will determine much of the data output you need to select during your Barracuda project setup.
- Solids entrainment? → Make sure you define flux planes.
- Erosion on walls? → Make sure you turn on the wall erosion model.
- Temperature profile? → Make sure to select thermal output variables.

Questions to Ask About Every Simulation You Run

What level of detail is required?

- Depending on what your goals are for a simulation, more or less detail may be required.
- Overall fluidization behavior might be captured well by a fairly coarse, fast-running model.
- Detailed flow behavior around small geometries can require a much finer grid, which could lead to significantly longer run-times.
- Is thermal required? Are chemical reactions important?

What amount of time needs to be simulated?

- Several time-scales could be important:
  - Fluidization / Hydrodynamics – how long does it take for the flow behavior to become quasi-steady?
  - Thermal – in some cases, thermal transients can be quite long.
  - Chemistry – is the chemistry fast or slow compared with other time-scales?
- Usually, we want to simulate something close to “steady state”, so keep in mind how long it will likely take to reach a “steady state” based on your initial conditions.

Questions to Ask About Every Simulation You Run

What simplifications can be made?

- Answer this question before CAD is created. In some cases, simplifications to the geometry of the unit can significantly alter the final CAD design.
- CAD simplifications can involve several types of simplifications
    - Exclusion of small or unimportant features
    - Making small features bigger if they must be included, to make gridding easier
    - Modeling small cylindrical features as square cross-sections for easier gridding
- Where can the model be started and stopped? Would some boundary condition simplifications make the model much easier to set up, without sacrificing the usefulness of the results?

The Simplified Model

In many cases, you can learn more about your system by running many coarse or simplified models rather than a single very detailed model.

The simplified gasifier that we will set up first is an example of such a model. It runs quickly and can be used to evaluate changes in overall operating conditions. It can answer big-picture "what-if" questions, such as:

- What if the superficial velocity is changed?
- What if the PSD of the bed is changed?
- What if the system pressure is raised from 1 atm to 1.5 atm?

More detailed models are useful if operating conditions are already well-defined, and if smaller variations in operating conditions need to be compared.

Coarse-to-Fine Resolution Studies

It is good practice with any CFD study, including CPFD Barracuda studies, to ensure that you have enough resolution to capture the physics of the system being simulated.

In Barracuda, this resolution depends both on the number of computational cells and the number of computational particles.

When running multiple simulations at different resolutions, it is best to run coarse variations first, since they will be the fastest. Then, move toward more fine-resolution cases, and compare them with the results of the already-run coarse simulations.

This strategy allows you to identify when you have enough resolution in the shortest amount of time.

Goals for Gasifier Training Models

Two distinct models for this training course.

The simplified model: isothermal, no chemistry, with simplifications to the geometry.

- From this model, we want to learn:
  - General fluidization behavior
  - Estimate entrainment of particles (both rate of entrainment and PSD of entrained particles)

The detailed model: chemistry and thermal are included, and the geometry is more realistic.

- From this model, we want to learn:
  - Are there any thermal “hot-spots” in the bed?
  - What is the gas composition exiting the gasifier?

Why a Grid is Needed

The grid defines the geometry of the simulation.

- The walls of the vessel being modeled are defined by the outer surfaces of the grid.
- A finer grid allows you to capture more geometric details.
- A coarser grid allows for faster simulations.

Spatial gradients depend on grid size

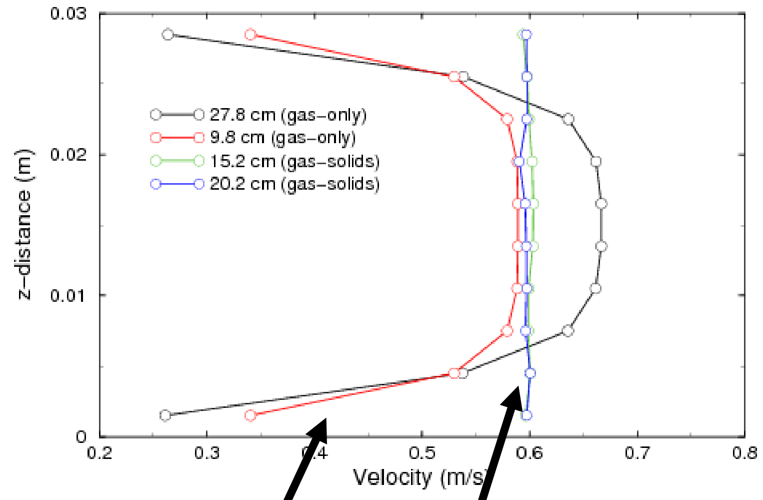
- All fluid field properties are calculated on the grid. The grid defines your computational cells.
- Particles are discrete, but their properties are interpolated to the grid for some calculations (inter-phase interpolation).
- A finer grid allows you to capture more details of the fluid-particle flow field, such as small bubbles or jets.
- A coarser grid allows for faster simulations.

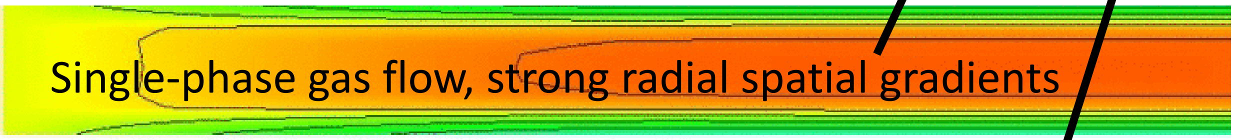
How much grid do I need?

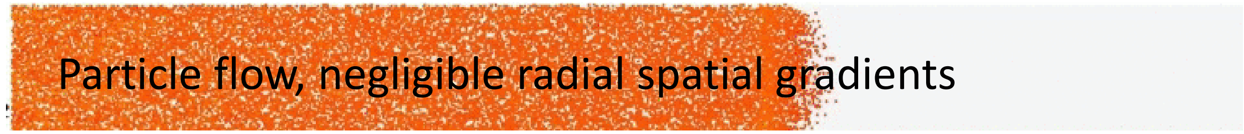
Single-phase fluid flow (e.g. air flow) often requires a fine mesh to resolve near-wall spatial gradients.

The presence of particles, however, tends to break up radial spatial gradients. Thus, when modeling particle flows in Barracuda Virtual Reactor, the computational grid can often be much coarser than a corresponding grid for a single-phase, fluid calculation.

The appropriate grid size for a particular geometry will be discussed further as the Barracuda New User Training class progresses.







CAD Requirements

For Barracuda simulations, we need a CAD model of the internal flow region.

- Calculations are being performed on the fluid and particles flowing in the vessel, and we need to define the flow region.

Many CAD designers will give you a thin-walled model of the vessel. But that is not what you want!

- Imagine that you fill your vessel with water and then freeze it. What we want is a CAD model of the resulting ice.

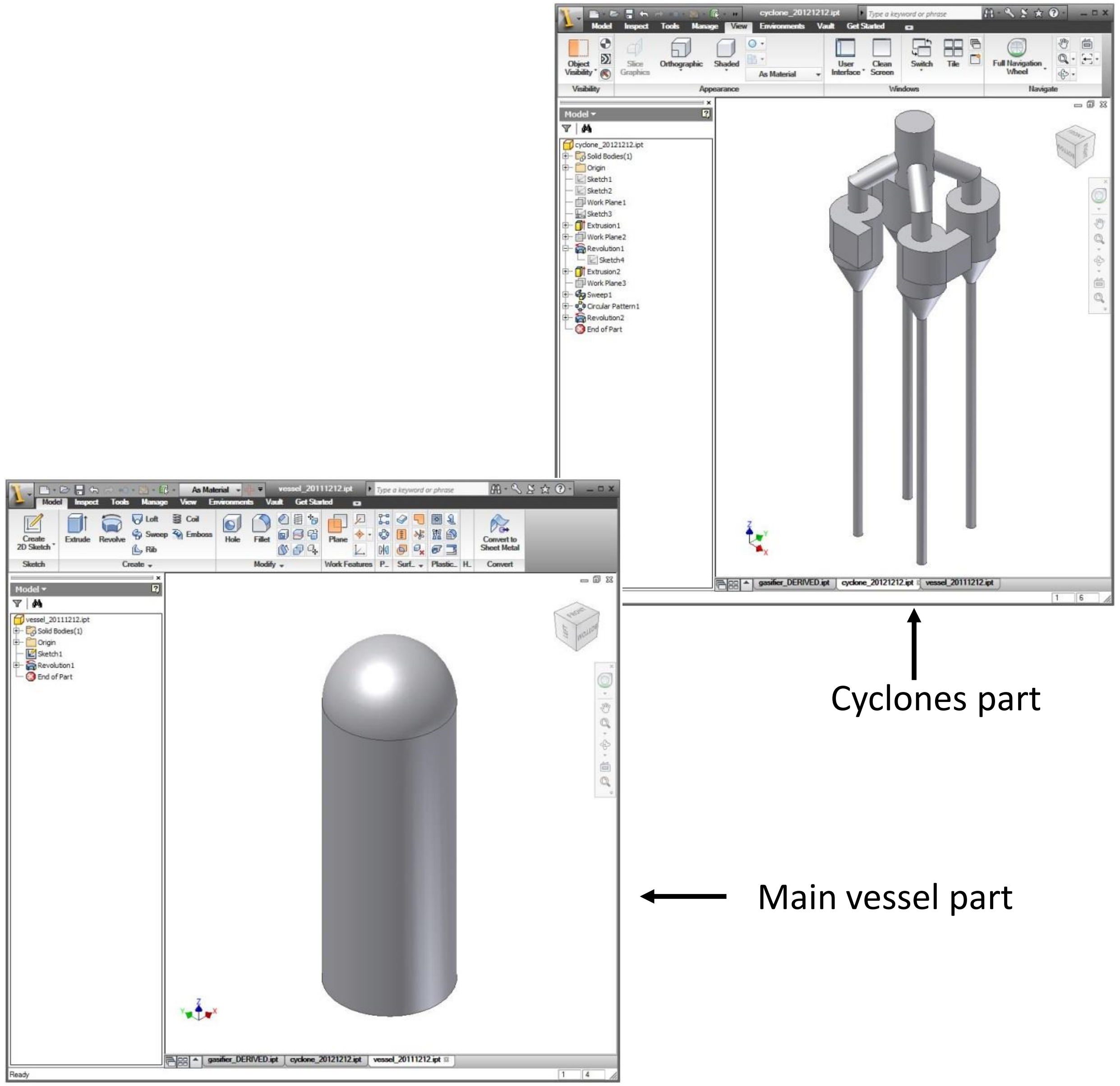
CAD – Parts and Assemblies

For CAD construction, we recommend using a parametric modeling system.

- Using such a system makes changing the CAD much easier, and changing the CAD is often necessary when simulating several variations of a given system.

The practice of using parts and assemblies is helpful for complex systems.

- Basic components are built as “parts” which are then combined into an overall “assembly”.



Cyclones part

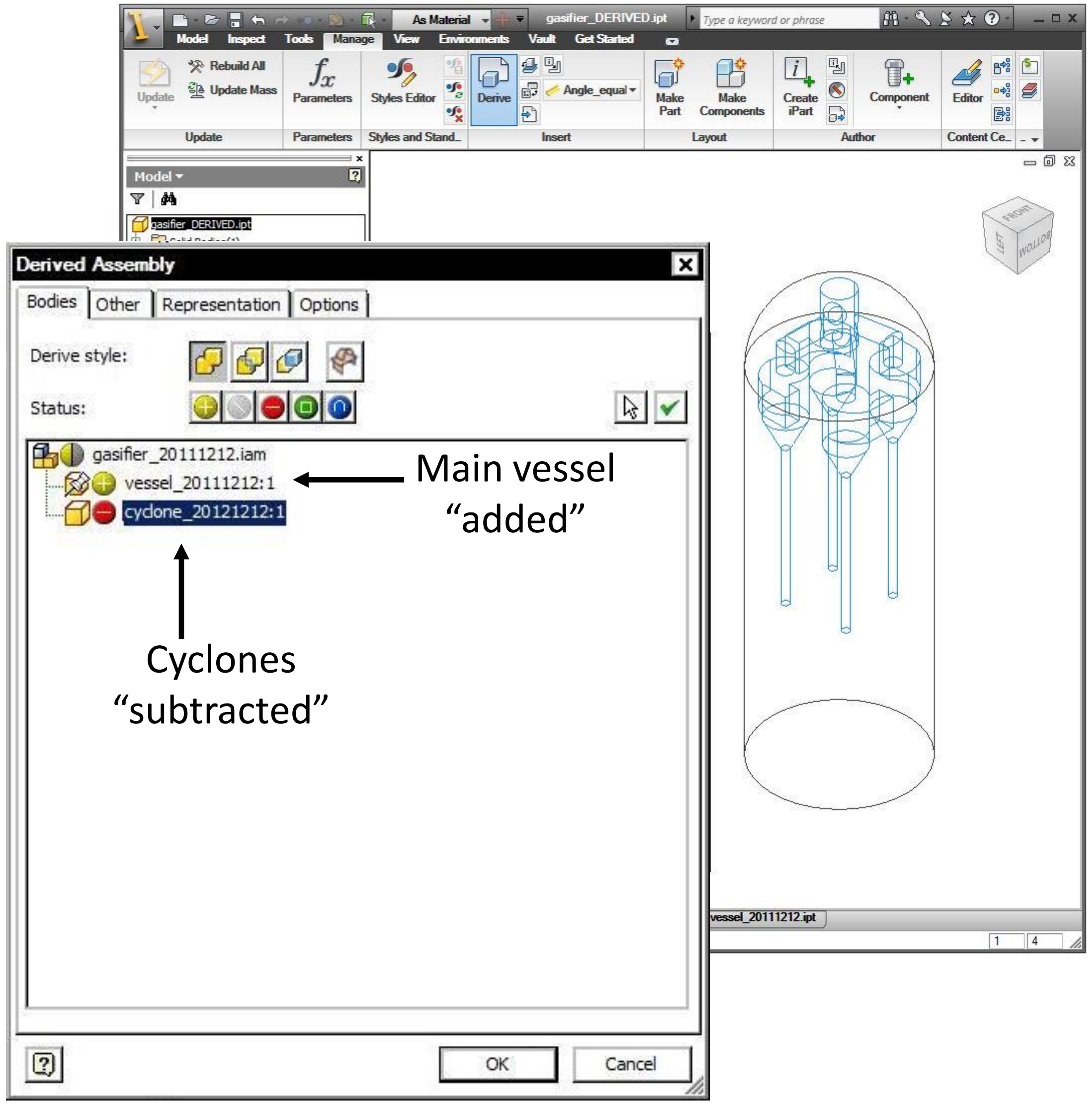
Main vessel part

CAD – Subtracting Internals

The final geometry is defined by subtracting individual solid parts from the assembly.

- The main vessel will typically be the only thing that you keep as a "solid", and any internal geometry will be subtracted from it.

In Autodesk Inventor, for example, one can use a "Derived Assembly" to select which parts are added and subtracted from the overall assembly.

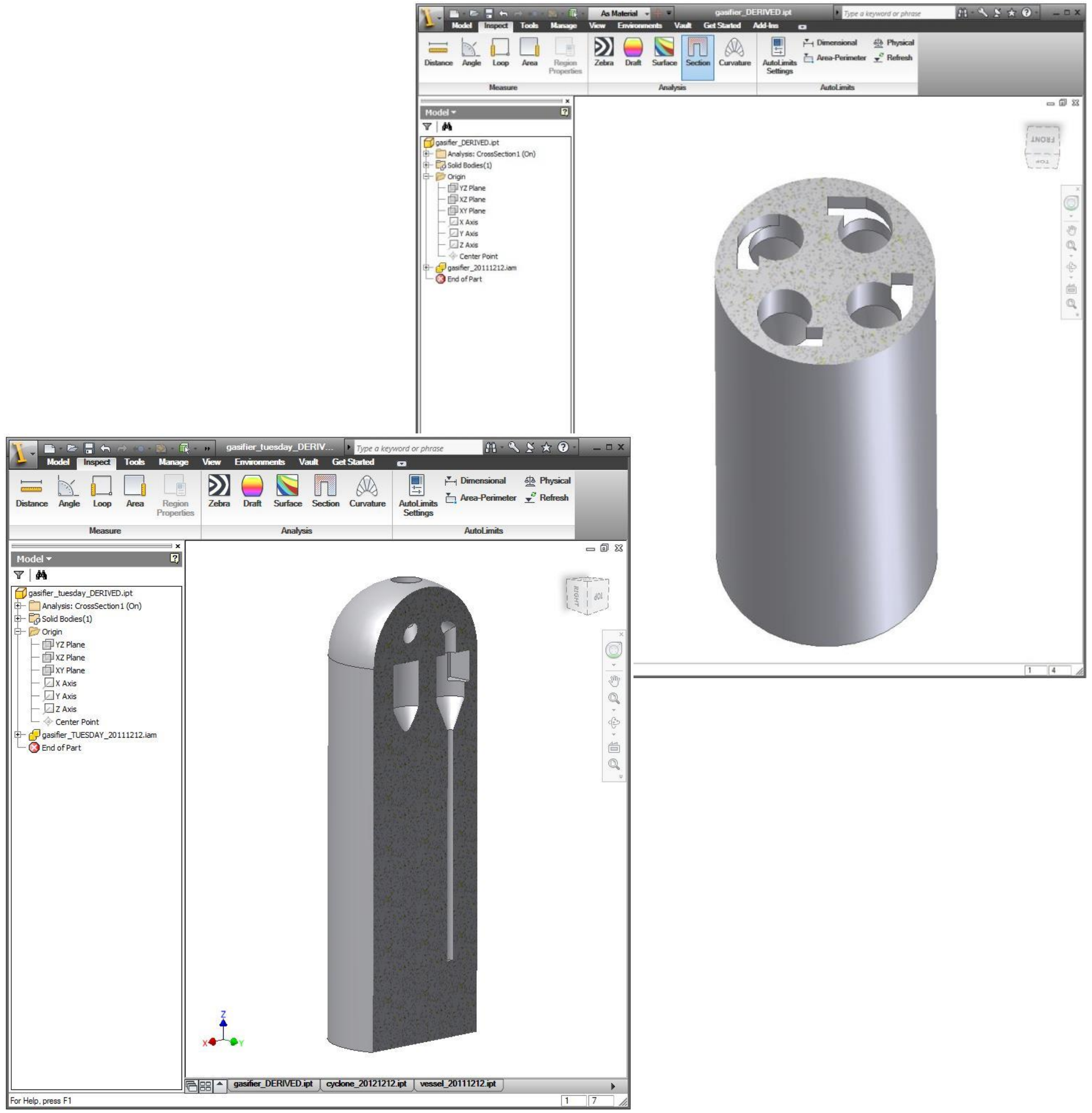


CAD – Final Part

The cutaway snapshots at right show that the final part is solid in all regions where fluid and particles can flow.

Internal geometry, such as cyclones, are subtracted from the main vessel.

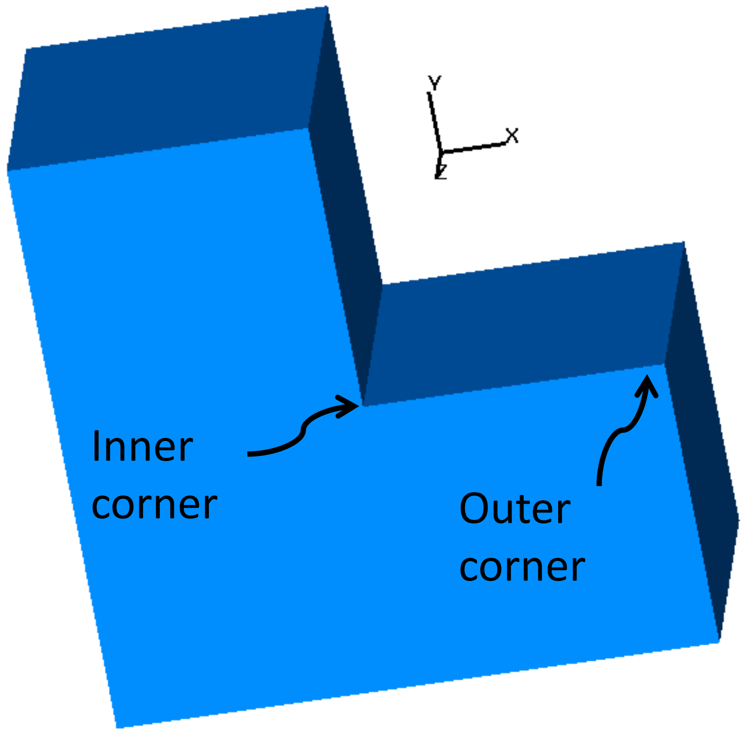
Once the final part is complete, it needs to be exported in STL format for use in Barracuda. Both ASCII and binary STL formats are supported, but binary is preferred.



Grid Generator Methodology Example 1: L-Shaped Geometry

The grid generator works by finding intersections of your defined grid lines with the STL geometry. It then "connects the dots" in 3-dimensional space to create the computational cells.

Consider the L-shaped geometry shown at right. This is a simple geometry, and it can be used to help us understand how the grid generator works. We will focus on the two corners indicated.



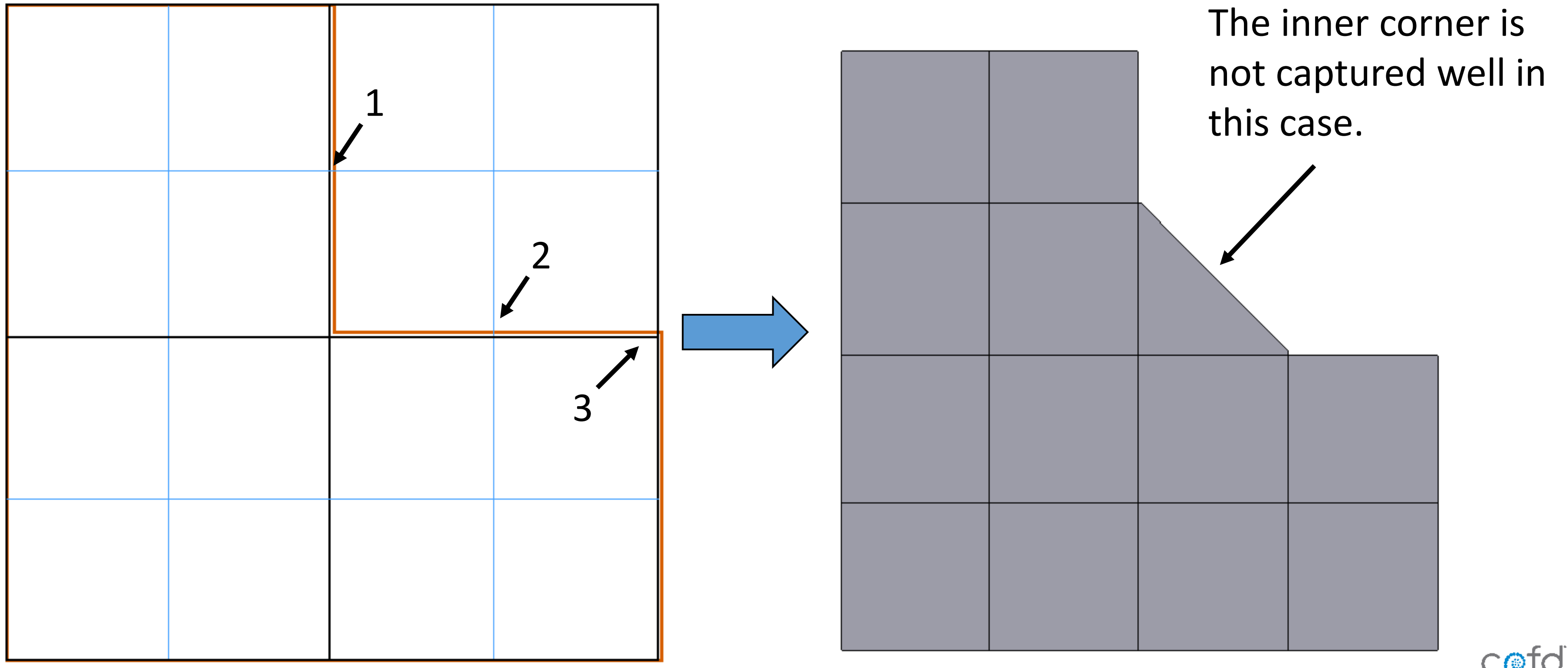
Three grid variations are shown next:

- Grid lines placed just inside the solid geometry.
- Grid lines placed just outside the solid geometry.
- Grid lines placed specifically to capture both corners well.

Grid Generator Methodology
Grid Lines Just Inside Geometry

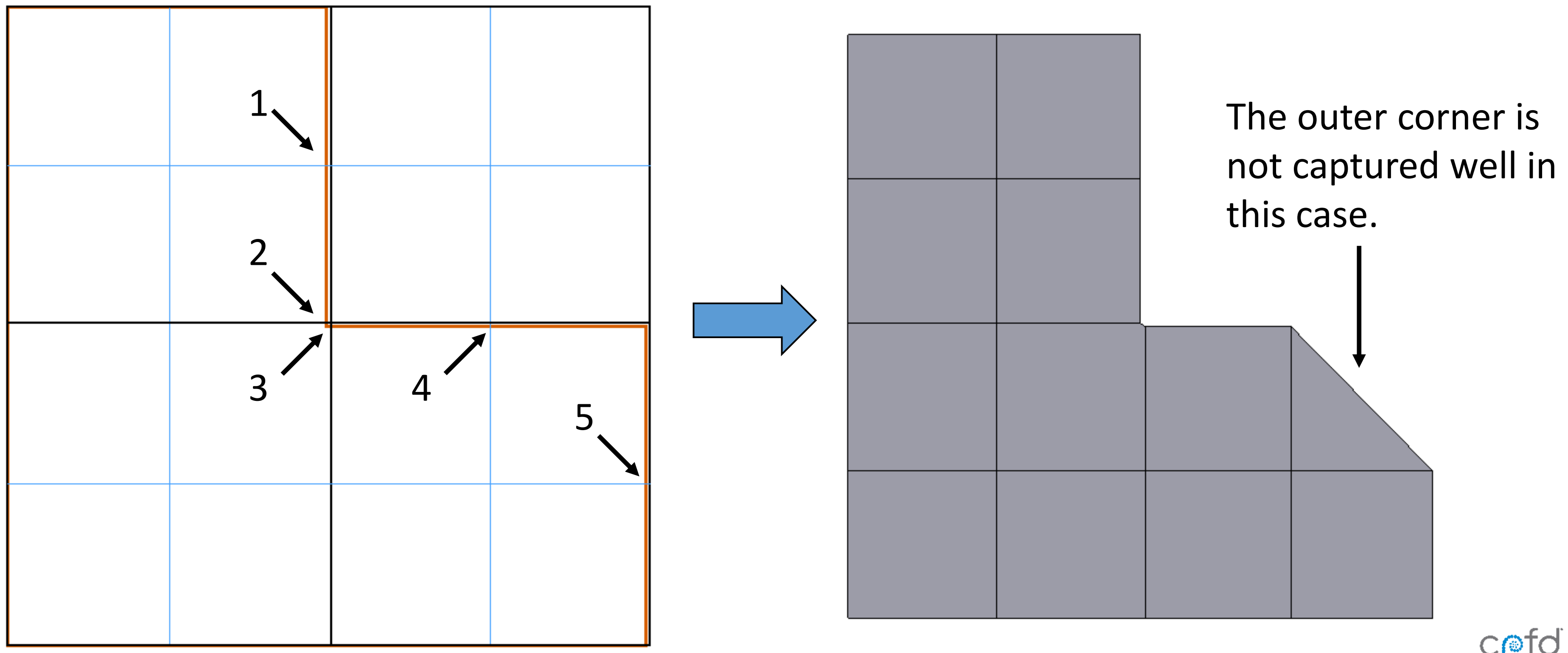
The grid generator searches for intersections of the grid lines (blue and black lines) with the STL edges (orange lines).

The intersections found in the case of grid lines placed just inside the solid geometry are shown here.



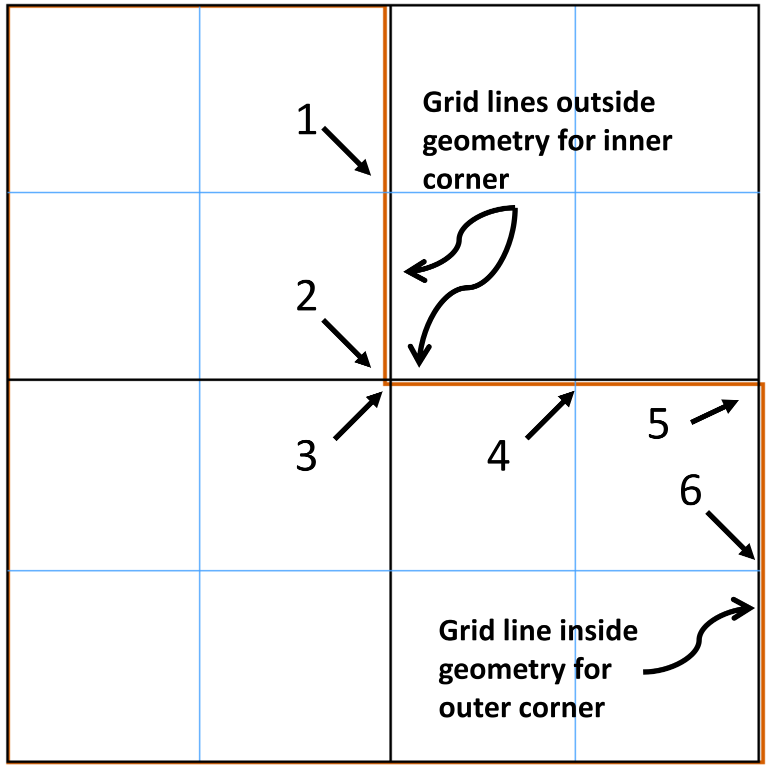
Grid Generator Methodology
Grid Lines Just Outside Geometry

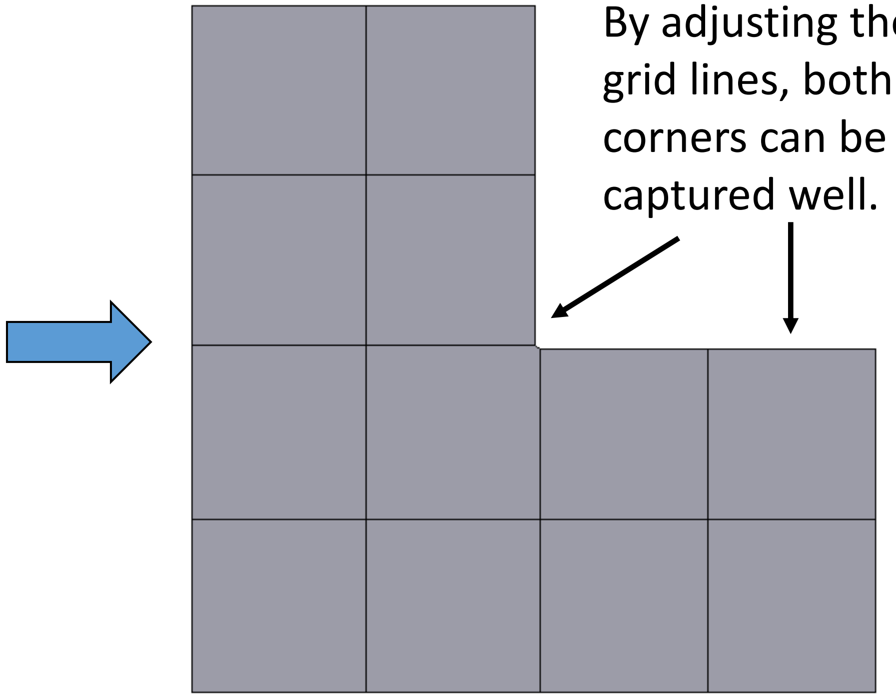
Moving the grid lines so they are just outside the geometry at both corners of interest changes the results. Now, the inner corner is captured well, but the outer corner is not.



Grid Generator Methodology
Capturing Both Corners Well

In most cases, you can capture both inner at outer corners simultaneously by placing grid lines in the correct locations (i.e. either inside or outside the geometry). The images below show how to define a grid that captures the L-shaped geometry well at both corners.



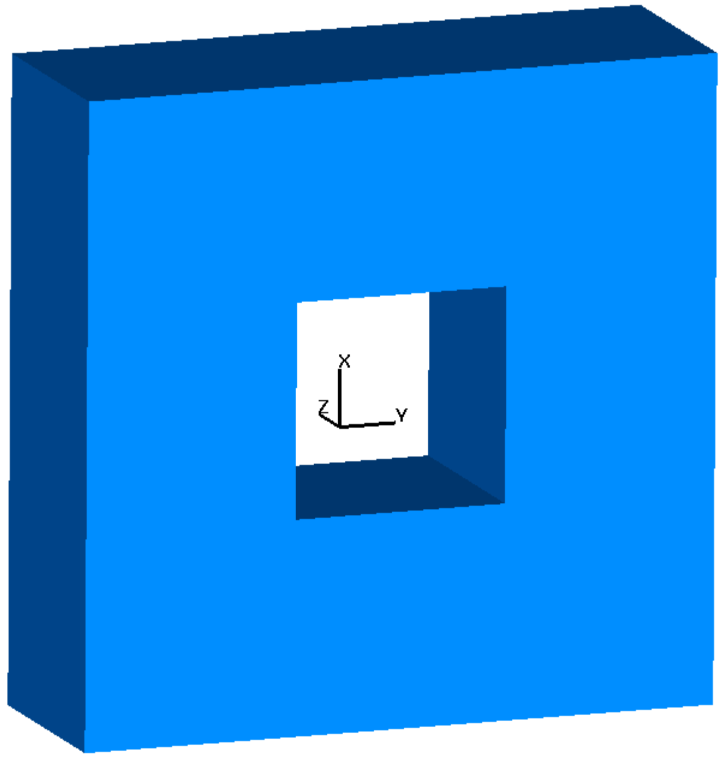


By adjusting the grid lines, both corners can be captured well.

Grid Generator Methodology Example 2: Block with Hole

A common situation when gridding geometries in Barracuda is that you need to capture "holes", usually internal structures such as cyclones or spargers that were subtracted from the vessel during CAD creation.

Consider the square block shown at right, which has a square hole removed from the center.



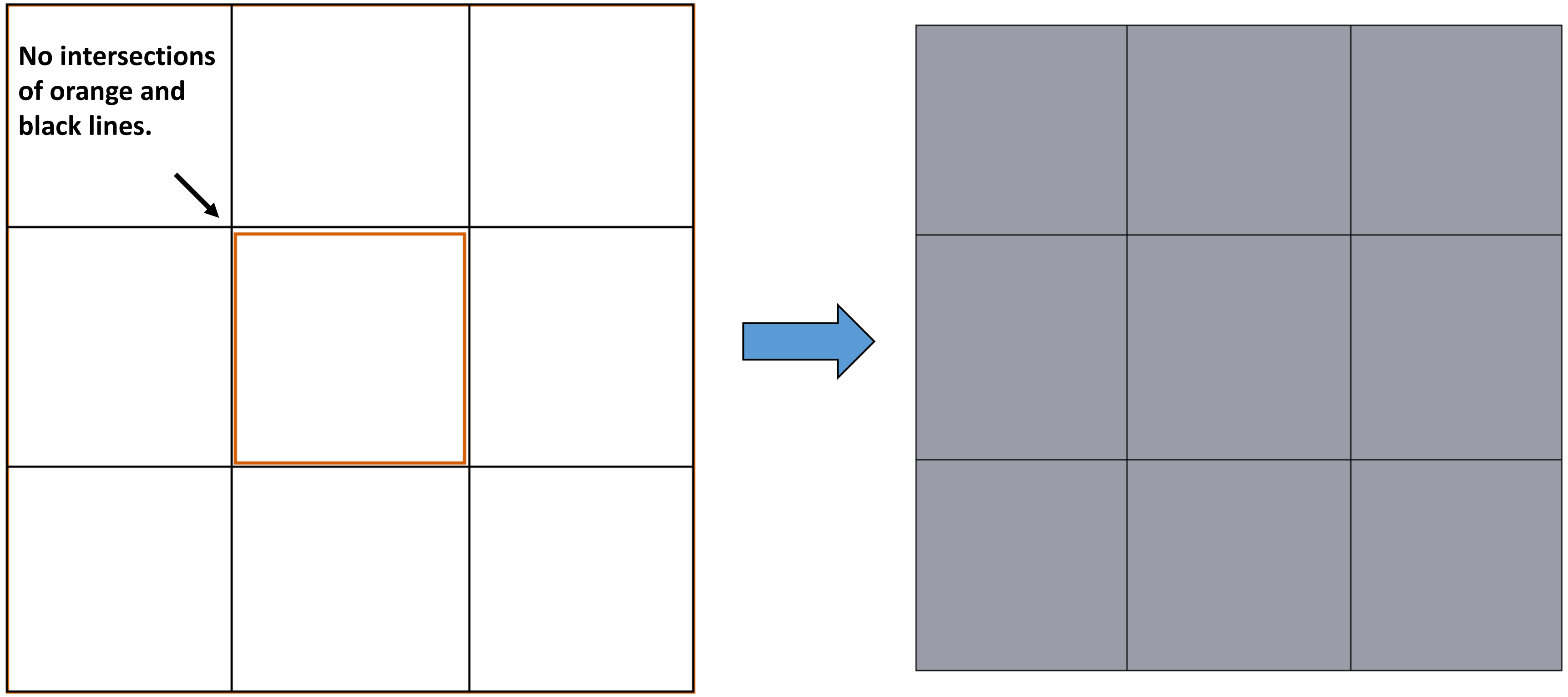
Three grid variations are shown next:

- Grid lines placed just inside the solid geometry (outside the hole).
- Grid lines placed just outside the solid geometry (inside the hole).
- Grid lines placed in a "cross shape" across the hole.

Grid Generator Methodology
Grid Lines Just Inside Geometry

If all grid lines lie inside the solid geometry (i.e. none cross the edges of the hole), then the hole will not be captured by the grid.

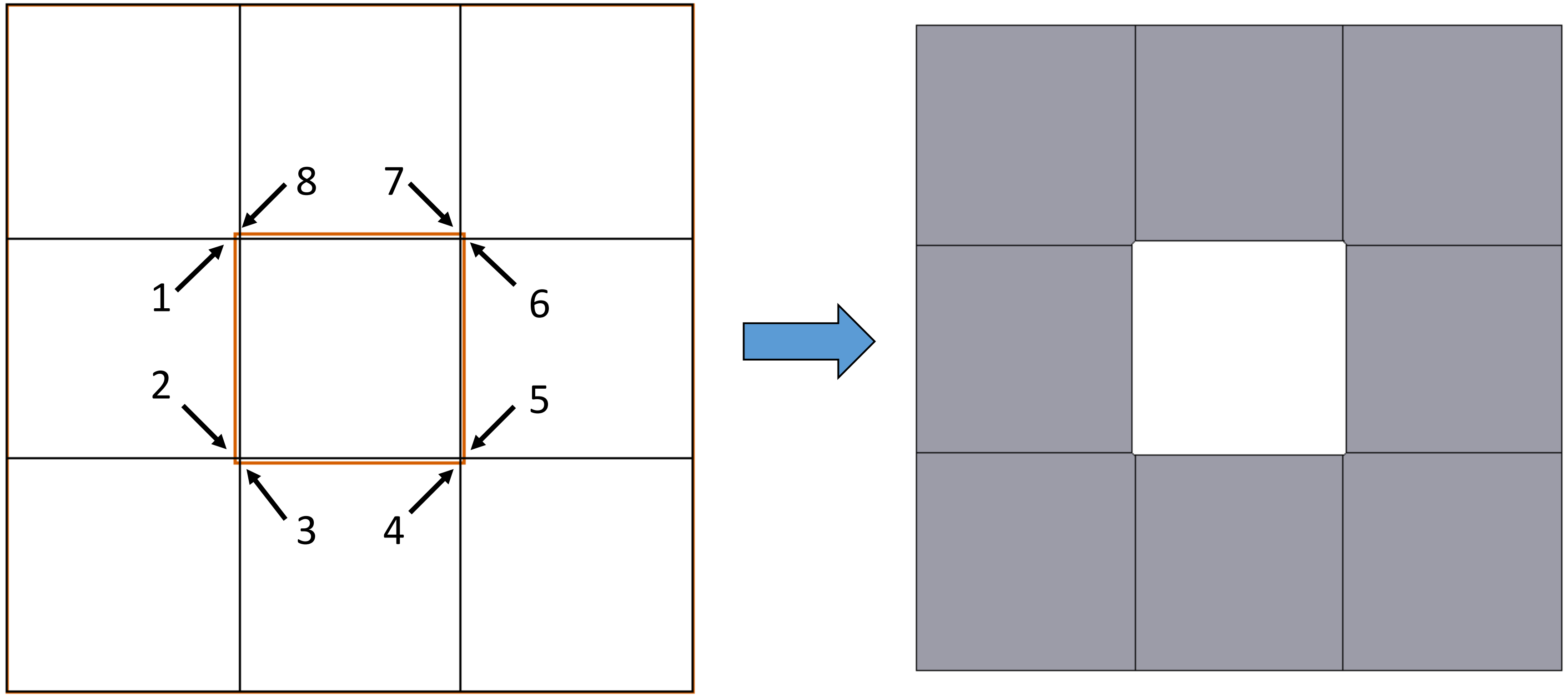
Since no grid lines intersected the edge of the hole, the resulting grid is completely solid.



Grid Generator Methodology
Grid Lines Just Outside Geometry

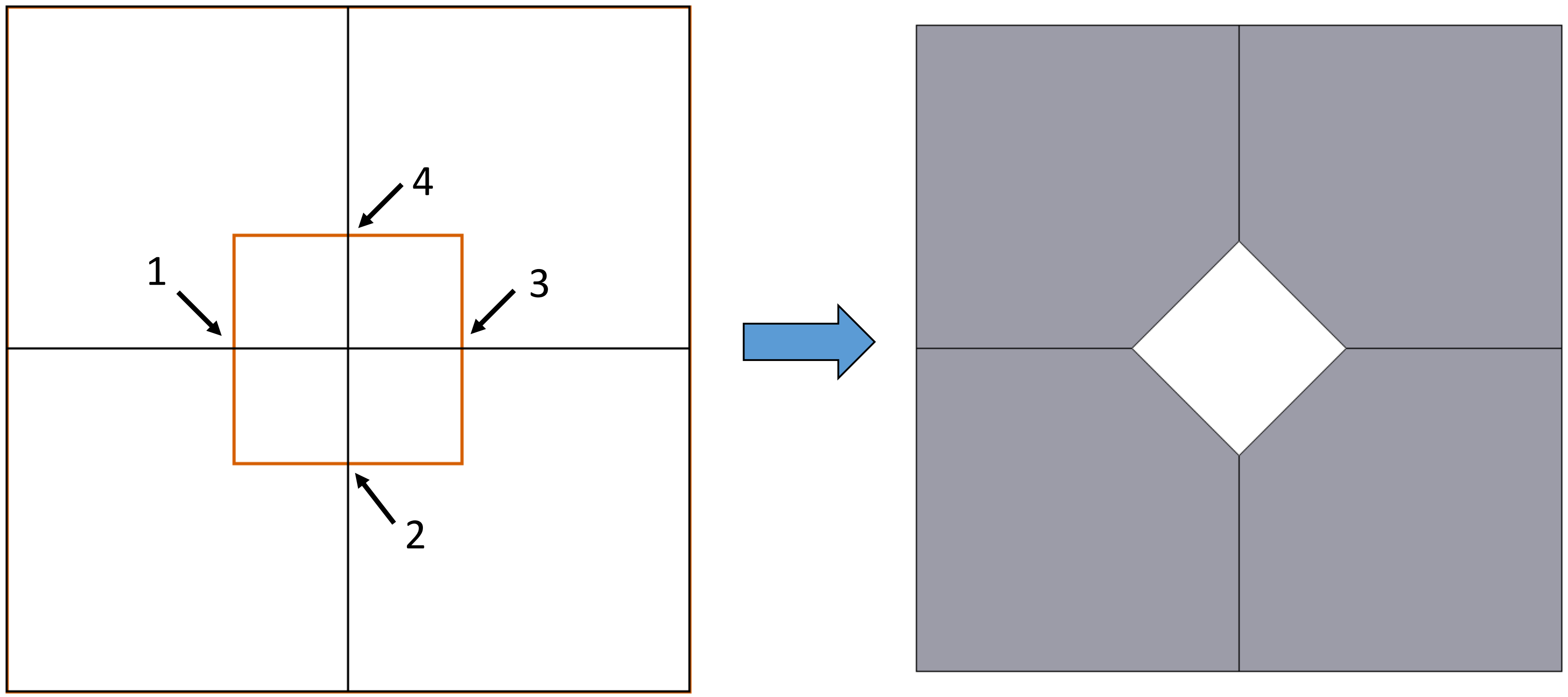
Since the grid lines are all just outside the geometry (i.e. just inside the hole), there are many intersections between grid lines and STL edges.

The resulting grid captures the hole very well.



Grid Generator Methodology
Cross Shaped Grid Lines

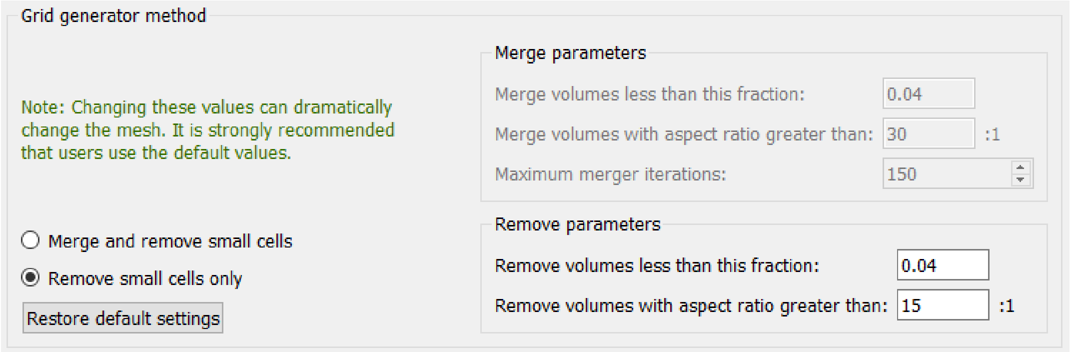
In some cases, a geometric feature is so small you can only intersect it with one grid line in each direction, such as the cross shape grid lines below. The resulting grid has a hole, but it is diamond shaped rather than the original square shape. This is because the grid only intersects the STL at four points.

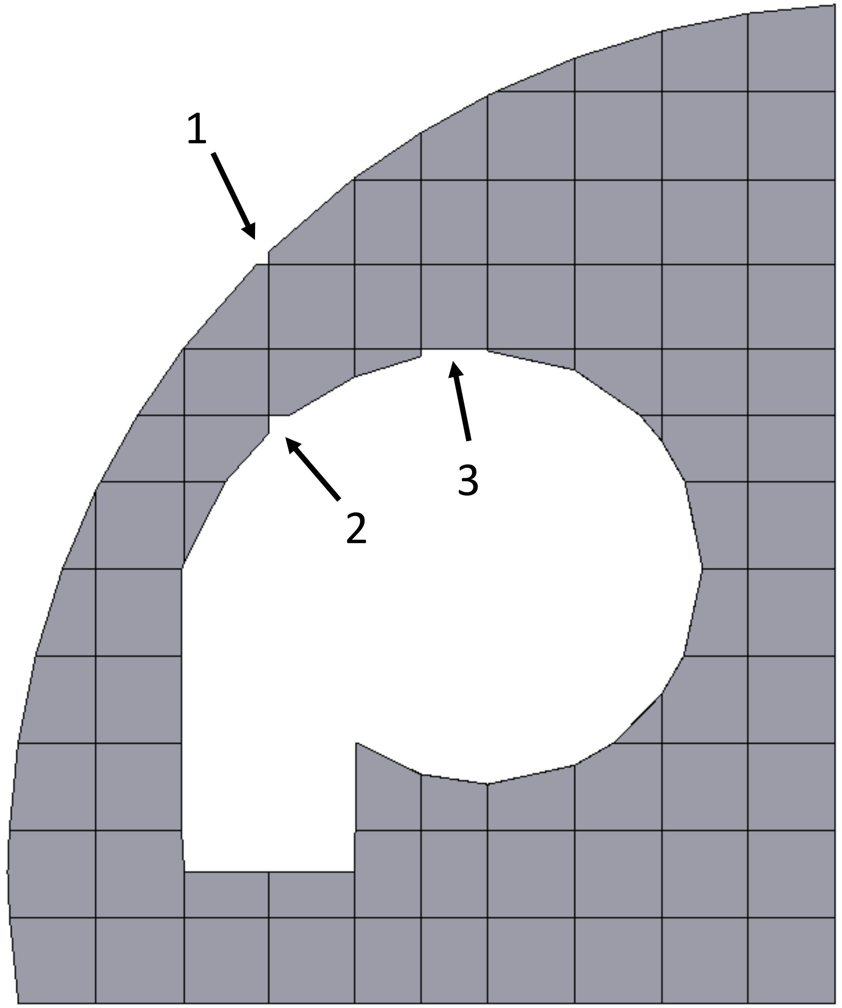


Cell Removal Criteria

Notice that there are some areas of the gridded geometry that are not as smooth as the original CAD.

Barracuda has certain criteria for removing cells from the grid. To see the default removal criteria, click Advanced Options in the Grid Controls tab.





Removing small cells helps to ensure numerical stability, so it is not recommended that you change the default values. Keeping smaller cells from being removed to make the geometry “look nicer” will not necessarily produce better simulation results. In fact, it could make the simulation run much worse.

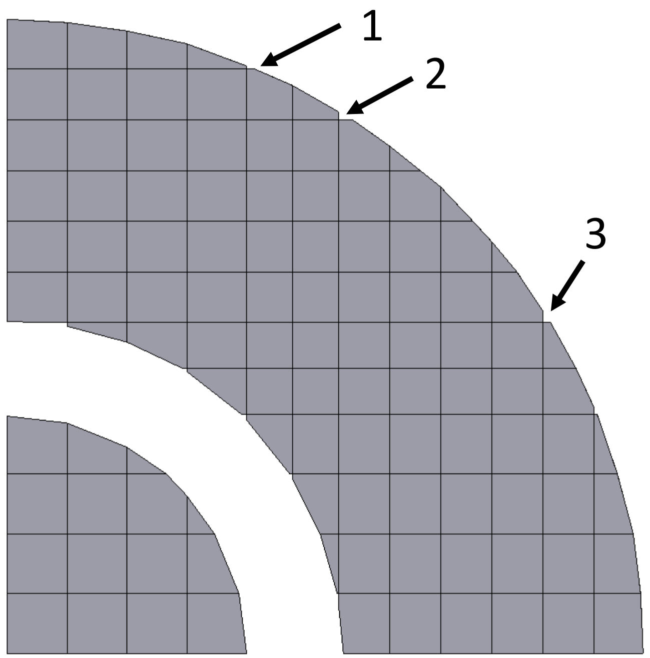
When to Use Merge Cells

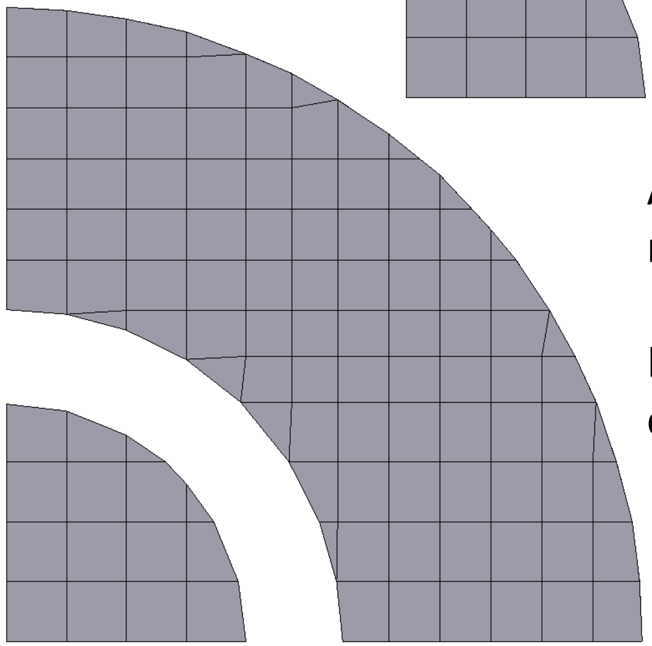
In some cases, the types of corners produced by cell removal can be detrimental to the physical calculations of particle flow.

When simulating the rotational flow of particles within a cyclone, for instance, particles would hit such corners and their momentum would be lost.

In such cases, using Merge and Remove within the Advanced Options can help. Cells are "merged" rather than removed by moving their nodes away from their normal Cartesian locations. The missing cell is thus avoided by creating cells that are not perfectly Cartesian in shape.

In general, the merge option should be used only when necessary.





Above: without merge cells

Left: with merge cells