# Best Practices

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# Training Objectives

- This presentation contains considerations and advice, based on the experiences of the CPFD Software engineering services and support groups

- The material in this presentation is intended to serve as a quick reference guide, rather than a complete working tutorial

- Much of the advice would be classified as "recommendations" rather than absolute rules.  These recommendations will save you time for many typical problems.

- Please ask your instructor about questions you may have about this material during the training class

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# Getting Started with a Project – Have a Good Process Description

- Before creating a Barracuda model, or even before creating an STL file, it is important to have a good understanding of the process you wish to simulate

- Information to include

    - Goal of the simulation – what problem do you wish to solve?

    - Geometry & region of interest ( a process diagram is very useful)

    - Operating conditions

        - All fluid flow boundary conditions

        - All particle flow boundary conditions (be careful to distinguish between fluid, particle and overall flow rates)

        - Anything else known about the system operation

    - Properties

        - Fluid properties

        - Particle composition, size distribution, behavior

    - Thermal behavior of fluids, particles and overall system

    - Chemical reactions and rates

    - Any data available for comparison including anecdotal information from equipment operators

    - A list of plots, images and animations desired

    - A list of assumptions

    - References for all of the above

- This may sound tedious, but will save you significant time in the long run for most complex projects

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# CAD Creation

- CAD input to Barracuda is via STL format

  - ASCII or binary STL options are both supported; binary is preferred

  - A fine resolution of STL triangles may not be required when exporting from the CAD software. Consider the typical cell size for your particular model

- The STL file must come from a 3D solid model of the internal flow region of interest

  - A thin-walled model of the vessel structure is not useful within Barracuda

- Many geometries are cylindrical in nature. If so, it is typically useful for the model origin to be centered at the bottom of the geometry with one axes up the middle

  - If the z-axis is pointing up (i.e. gravity in the –z direction), mouse rotations will be most natural in GMV

  - If the z-axis is not pointing up, you may consider using the **Ctl-3 -> Use virtual trackball** option for mouse rotation in GMV

# CAD Creation Continued

- Consider carefully how to handle small geometric features in large vessels

- Some features can be neglected (e.g. individual sparger shrouds when studying overall entrainment in a large vessel)

- Some features may be made larger in the CAD to facilitate gridding (e.g. a wall separating the vortex tube from a cyclone body)

- Some features must be left as is.  This is true if the actual size is relevant to the objectives of a simulation (e.g. individual sparger shroud when studying jet penetration).  In such cases, your options include:

    - Run a fine model of the overall vessel.  The runtime may be extremely impractical if the characteristic length scale of the feature is orders of magnitude smaller than a characteristic vessel dimension

    - Run a local model of the region in the immediate vicinity of the small feature.  Boundary conditions for this may be extremely challenging to define

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# Model Size

- Barracuda is used to simulate a wide variety of fluid-particle flow problems for a wide variety of industries. Spatial dimensions, flow rates and the time required to reach a quasi-steady solution can vary by several orders of magnitude. Thus, it is not possible provide rigid guidelines for computational cell and particle counts.

- However, it is important to remember that the CPFD method obtains solution resolution from both the Eulerian (grid) and Lagrangian (discrete) phases – thus the number of cells in a CPFD grid is typically much lower than that in a CFD grid, where solution resolution is primarily tied to grid resolution alone. Many Barracuda projects can be run with:

  - Between 50,000 and 300,000 real computational cells

  - Between 500,000 and 5,000,000 computational particles

- Be aware of the effect of model size on calculation run time

  - Doubling the number of computational particles for a given grid, can roughly double the run time

  - Doubling the cell count will automatically double the number of computational particles as well. Doubling the number of cells thus results in problem with 3-4 times the original run time

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# General Advice – Grid Definition

- Check STL units.  Incorrect assumptions here are a common source of error.

- Do not put a large cell next to a small cell.

  - This is bad practice with any CFD.

- Avoid widely varying cell sizes on a global scale.

  - Try to keep the largest cell size < 3.0 times the smallest cell size in any linear direction

  - For a CPFD calculation, widely varying cell sizes may hinder the solution speed or stability in some cases

- Check your cell count before running the solver.   The cell count can be found near the end of the grid.log file.  Look for the **Total number of real cells**.  More useful information may be obtained by running many smaller problems in the same time it takes to run one large calculation

```
Summary of cells and cell volumns
----------------------------------
Grid dimensions nx, ny, nz = 24  34   158
Total number of all cells  = 128928
Total number of null cells = 81442
Total number of real cells = 47486
```

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# General Advice – Calculation Set-Up

- Consider running a fast-running approximation before running a detailed calculation.  Much can be learned from these "workhorse" models.

- When initializing particles in the domain, use the automatic number of computational particles whenever possible.  A "medium" or "medium-high" value often works best.

- When using particle feed at boundaries, ensure you are using a good number of computational particles

  - Check visually in GMV.  You want some statistically significant number of particles in each cell.

  - Perform some analysis.  A conservative algorithm is to divide 50 by the volume fraction you hope to resolve with the feed particles:

    - E.g.  Particles are flowing in at 50% by volume.  50/0.5 = 100.  Use 100 as the number of computational particles at feed.

    - E.g. You have a dilute feed stream coming in at 1% solids by volume  50/0.01 = 5,000.  Use 5000 as the number of computational particles at feed.

- Consider initializing particles slightly below close pack, rather than at close pack.  This is easier on the solver.

- Avoid placing a boundary condition in the location of a strong gradient.  It is not always possible to avoid this

- Unless you are trying to resolve shocks, ensure your initial pressure and boundary pressures agree

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# General Advice – Calculation Start-Up

- Are your boundaries specified correctly?

  - Especially check particle boundaries carefully. The local, transient physics of a problem may prevent particles from entering at the specified rate. Always plot particle mass flow rates at inlets to ensure the desired mass flow is achieved. Check this over time as well.

- Are your particles initialized in the right location?

- Check the number of computational particles in the calculation. This can be found:

  - In POPULATION* files. One is written at time zero. Others are written whenever restart files are output.

  - By opening GMV at the command line. Look for the number of tracers.

- Check how the number of computational particles changes with time.

- Are your flux planes and transient history points properly defined?

- Does the Gmv.00000 file contain all the information your desire?

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# General Advice – Calculation Start-Up Continued

- Check velocities early on.  Incorrect boundary conditions will often be apparent when checking velocities.

- Check your time step

    - Shortly after startup

    - After the calculation has been running for some time

- Check the number of GMV files produced

    - Too few, and you won't have smooth animations

    - Too many and you'll fill your hard drive!

- Do you have enough disk space to run the calculation?

    - Check how the directory size grows after a day or so.

- Have someone else review your work.  It's OK if the other person is not a Barracuda user – just explain to them your process sheet and show them your model.

# General Advice – Data Output

- It is usually a good idea to use flux planes liberally:

- Use at every boundary

- Put several across your entire domain

- If using multiple gaseous species, be sure to activate the gas species output option on flux planes, particularly at the model exits

- If you want to track PSD crossing a flux plane, be sure to activate the **Subdivide by radius** option

# General Advice – Thermal Calculations

- When running thermal calculations:

- Check temperatures carefully on setup:

    - Initial fluid temperatures

    - Initial particle temperatures

    - Boundary temperatures.

- Check material properties over the range of expected temperatures.

    - For specific heats, do not operate near the low/high split of the two curves

- Consider carefully wall effects.

    - Adiabatic?

    - If a wall temperature is known, where is that temperature (inside, outside). Consider appropriate heat transfer coefficients.

    - If a heat flux is known, you can change your wall temperatures interactively while monitoring the heat flux reported.

- Consider physical time-scales to equilibrium. For a large fluidized bed of solids, the thermal time-scales may be much longer than the hydrodynamic time-scales.

# General Advice – Calculations with Chemistry

- When defining a reacting flow problem, check the molecular weights of all materials. Most material property databases average isotopes. When performing chemistry, it is important to conserve mass. This is done by computing the behavior of the most abundant isotope (i.e. rounding molecular weights).

- Check heats of formation of all reacting materials carefully.

- It is a good idea to obtain all kinetics from a single experiment whenever possible, rather than "mixing and matching" from various sources

- Check units on reactions very carefully

- If using discrete particle chemistry, ensure the rate you input is per particle, and not per unit volume

# General Advice – Calculations with Chemistry Continued

- It is strongly recommended to check your kinetics in a simple geometry (usually a 1-D tube) before including in a complex model

- Look at the chemistry summary in the "info.log" file. This is often a good way to catch errors.

- The calculation can be started with chemistry off; the reactions can be toggled on at a later time. However, do not use this feature if reactants for fast reactions are building up in the system (i.e. are you trying to model an explosion?). Generally it's best to start with your chemistry on from time = 0.

- You will generally want gas species information through various flux planes when modeling chemistry.

  - Be care to select output formats that are meaningful to you (mass fraction, mole fraction, mass concentration, mole concentration)

- Time averaged gas species information is often desired when modeling chemistry.

# General Advice – Post-Processing

- Begin post-processing as soon as possible after your calculation is running.  The calculation need not be complete.  This will ensure everything is set up correctly and all desired data is available.  If there is a problem requiring a change in setup, it is better to find this out early, rather than after the calculation has completed.

- Practice scripting your analysis.  Even if you are not overly comfortable with this yet, this skill can be learned and will greatly increase your efficiency using Barracuda.  At a minimum, learn to use the BATCHMOVIE.sh script.

# General Advice – Miscellaneous

- If running grid resolution studies, run your coarser models first

- Check particle resolution, particularly when studying the behavior of a size range representing a small portion of the overall PSD range

- If your particle equations are having difficulty, try:

    - Using more computational particles

    - A more uniform grid

    - Removing more small cells during grid generation

- If modeling very small particle, consider if other physics are important which are not directly computed by Barracuda.  For example, small particles tend to cluster or agglomerate.  It may be important to use an agglomeration drag model when modeling small particles.

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# General Advice – Miscellaneous Continued

- Define boundary conditions as transient (.sff files) even if you do not intend for them to change with time.  This will allow you to change this interactively, or on restart, if later desired.

- Use recommended file extensions (.sff for input files, .sff for PSD tables, etc.).  This will facilitate support and archiving

- Start flux plane names with either "Flux" or "FLUX".  This will facilitate support and archiving.  Also, the file viewing defaults in Barracuda look for flux plane files following these naming conventions.

- Never rerun your grid generator in the same directory after starting the solver.  If you do so, your results will be lost!

    - If this happens contact support – there is sometimes a way to recover your results.

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# Restarting Barracuda

- It is possible to restart a Barracuda calculation from a restart (IC) file

- To raise the **Restart** dialogue, click on **Restart Solver** on the **Run** page

- An **IC** file name must be selected

- Other information should only be entered if you want that information to change from the current run

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# General Project Management

- Barracuda creates many output files as it runs.  Be sure to run each calculation in a different directory.

- When running multiple simulations for the same project, be sure to uniquely name each directory

  - If the names are not fully descriptive of the contents (run1, run2, etc.), then be sure to keep a text file containing notes and explanations.  For example:

    - Run1 – baseline simulation using process conditions contained in process_sheet_2012_01_23.doc

    - Run2 – based on run1, but regridded cyclone inlets.  This is the case reported in the baseline report

    - Run3 – based on run2, but increased superficial velocity 15% to study effect on erosion

- Be mindful of disk space as you run

  - Check the amount of space remaining before starting a new calculation.  Look at other directory sizes to estimate roughly how much space is needed.

  - For very long running calculations, check space periodically

  - Archive files as needed

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# Additional Calculations Started from Time Zero

- When starting additional calculations, based an existing calculation, certain files must be copied to the new directory.

- A minimum set of files includes the following.  In this case, the grid will need to be regenerated in the new directory:

  - Project file (*prj)

  - Transient input files (*sff)

  - Particle size distribution files (*sff)

  - CAD (*stl, *STL)

- If you do not need to change your grid, you may copy the related grid files as well:

  - VIEWGRID.gmv

  - 00* (note these files are created when the grid generator runs and must reside in your working directory)

- In general, it is a good idea to also copy the following:

  - Any GMV attribute files (*attr)

  - Any analysis scripts you have written (*sh)

  - Any files referenced in the analysis scripts (*par, others?)

- Optional short-cut.  Some of these files are compressed and bundled using the Create support file button on the Post-run dialogue.  If you are familiar with Linux, you may extract these files to the new directory.  You will need to regenerate your grid, as it is not bundled with the support file.

# Additional Calculations Restarted From Other Calculations

- It may be desirable to restart additional calculations from an existing calculation, rather than starting them at time zero.  If restarting:

- First copy files from the original directory following instructions from the previous page

- Additionally copy the following:

    - The desired restart file (starts with IC_)

    - Flux plane files (FLUX*, Flux*)

    - history.log

    - Other output files (*dat*)

- Be sure your grid is generated in the new directory before restarting

# Additional Calculations Restarted From Other Calculations

- Next change process conditions. Note, items that can be changed on restart are shown on the **Restart Calculation** window. Any other changes made to the project file will not be reflected in the restarted calculation. Typical changes include:

    - Boundary conditions. These must be changed in the transient (*.sff) files. If these are changed, click on **Reread BC input files**.

    - Particle size distributions. These must be changed in the text files (*.sff). If these are changed, click on **Reread BC particle size distribution tables**. Note, this will not affect particles already in the calculation domain – only particles fed into the system after restart will have the new size distribution.

    - Turning on thermal or chemistry

- Be extremely careful when changing process conditions on restart. Take careful notes on what was changed and when. It is easy to confuse calculation results when using this technique.

# Archiving Project Results

- After completing a project, it may be desirable to archive results, in order to free disk space on the computer

- When archiving, it is recommended to save the following as a minimum set:

  - Files needed to rerun (Project file (*prj), Transient input files (*sff), Particle size distribution files (*sff), CAD (*stl, *STL))

  - Grid (VIEWGRID.gmv, 00*)

  - Some Gmv files (maybe every 2nd, 10th, 50th or 100th)

  - Restart file (at least final IC file)

  - Other output files (history.log, flux planes (FLUX*, Flux*), transient data (*data*), 2D data (*dat))

  - Post-processing files (any scripts created and files referenced (*ipynb, *py, *sh, *par), GMV views (*attr))

  - Images, animations and plots (*jpg, *png, *eps, *mpg, *avi, *sav)

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# Contacting Support

- If you have questions about this material, or a specific question, please contact the CPFD Software support team ([support@cpfd-software.com](mailto:support@cpfd-software.com))

- If your question relates to a specific project, please include a "support file" if possible

- To create the support file click on the  button on the **Post-run** dialogue.  Be sure to include the CAD.