

**ASCOMP**

MULTIPHASE FLOW SCIENCE AND TECHNOLOGY

# Trans**AT**

## Release Notes

Version 5.3.1.5.1

# AT

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This document summarizes the latest developments brought into TransAT since the previous release. It also reports the changes and corrections to the currently known limitations including updates from revision 5.2.

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## 1 Updates since release 5.3

### 1.1 Patch 5.3.0.1

- **TransAT**
  - Fix for massflux printed by section output for single phase flow and Level-Set method
  - Fix for void fraction calculation at the pressure outflow boundary for homogeneous model
- **TransATUI**
  - Improvements for handling checkbuttons, value inputs, text buttons
  - Improvements for handling sliders
  - Bugfix for resizing blocks with BMR
  - Turbulent dispersion activated automatically with RANS

### 1.2 Patch 5.3.0.2

- **TransAT**
  - Fix corrupted cantera library
- **Installer**
  - Fix for port settings extraction in pre-set TransAT environment on Windows

### 1.3 Patch 5.3.0.3

- **TransAT**
  - Improvement of k-epsilon model wall shear computation
  - Fix to correctly stop restarted parallel steady simulations at convergence
  - Fix for velocity outflow in z-direction using immersed surfaces

### 1.4 Patch 5.3.1.1

- **TransAT**
  - Integration of SArP convergence control module
- **TransATUI**
  - Update of graphical user interface workflow
  - Improvement and reorganization of inputs
  - Restructuring of interface for loading object files

- **Installer**
  - Inclusion of specific Python version for TransAT
  - Fix for manual selection of MPI executable

### 1.5 Patch 5.3.1.2

- **TransAT**
  - Clean exit of simulation for simulation aborted early due to physical inconsistency in initial conditions
- **TransATUI**
  - Fix display inconsistencies in Geo tab
  - Fix Geo tab scroll bars
  - Fix wrongly displayed units in Create Shape tab

### 1.6 Patch 5.3.1.4

- **TransAT**
  - Setting of inflow void fractions from data files
- **TransATUI**
  - Handling of void fractions in inflow from data file window

### 1.7 Patch 5.3.1.5

- **TransAT**
  - Setting of various multiphase flow topologies as inflow boundary conditions
    - Horizontal Slugs
    - Vertical Slugs
    - Annular Flow
    - Stratified flow
  - Reorganisation of VTK-output and folder structure inside RESULT folder
  - Improved handling of embedded objects for
    - touching objects
    - object surfaces close to domain boundaries

- [TransATUI](#)
  - Handling of multiphase inflow topologies in inflow properties window

## 1.8 Patch 5.3.1.5.1

- [TransAT](#)
  - Fix for VTK-output for parallel processing
  - Fix for lower-case file names in boundary conditions

## 2 Update Highlights

### 2.1 Simulation Information

The execute tab of **TransATUI** where simulations are run has been extended as shown in Figure 1.



Figure 1: Execute Tab

A new panel, "Runtime information", which is displayed in Figure 2 has been added. It contains information about:

- the running (or previously run) simulation timings including estimates for the remaining simulation time (1)
- detailed colored information about inner/outer loop convergence for each variable (2,3) as shown in Figure 2.

The following information is also available in the information panel:

- overview of all info-, warning- and error-messages of the simulation
- license information

Some changes have also been introduced to the simulation screen output to make residual output easier to read. The residuals are now displayed using a color code to highlight the convergence status and problems for equations that are solved for. An example is displayed in Figure 3.

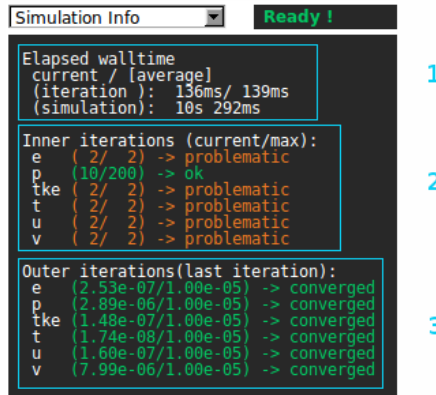


Figure 2: Simulation Information Panel

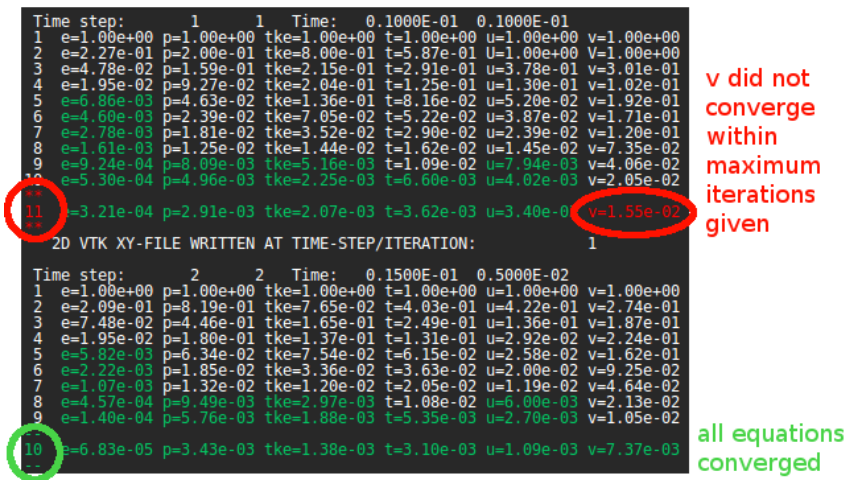


Figure 3: Simulation screen output

## 2.2 Initial conditions

In TransAT versions that predate this release, it was only possible to set initial conditions through a C++ file – `initialconditions.cxx`. This is a powerful and flexible way to set up initial which is quite advanced. It requires the compilation of C++ files which can be troublesome to do on some systems due to installation issues.

To alleviate potential issues and simplify the simulation workflow, new types of initial condi-



tions that do not require any compilation have been introduced. They complement the advanced initial conditions with a C++ file. They can directly be set in [TransATUI](#) or through an xml file – `initialconditions.xml`.

Overall, there are now three types of initial conditions in [TransAT](#):

- basic initial conditions which can be set directly in [TransATUI](#)
- user-defined initial conditions which can be defined by editing `initialconditions.xml`
- advanced initial conditions which can be defined by editing `initialconditions.cxx`

The basic initial conditions can be of two types:

- constant: initialises a variable with a constant value over the domain
- automatic: only available for pressure and velocity components in incompressible simulations; sets divergence-free initial velocity profile and initial pressure distribution based on source terms

The user-defined initial conditions are particularly useful to define interfaces between fluids modelled with the Level-Set method from a set of predefined shapes. An example with two spheres initialised with user-defined initial conditions is shown in [Figure 4](#). The corresponding xml file is displayed below:

```
<?xml version="1.0"?>
<initialconditions version="5.3">
  <VARIABLE variable_name="Level-Set">
    <method type="string" value="Userdefined">
      <attribute name="sign" value="negative" />
      <object type="sphere">
        <attribute name="center">
          <coordinate direction="x" value="0.00225" />
          <coordinate direction="y" value="0.0015" />
          <coordinate direction="z" value="0.002" />
        </attribute>
        <attribute name="radius" value="0.001" />
      </object>
      <object type="sphere">
        <attribute name="center">
          <coordinate direction="x" value="0.00175" />
          <coordinate direction="y" value="0.0038" />
          <coordinate direction="z" value="0.002" />
        </attribute>
        <attribute name="radius" value="0.001" />
      </object>
    </method>
  </VARIABLE>
</initialconditions>
```

```
</VARIABLE>  
</initialconditions>
```

More details can be found in the User-defined Initial Conditions section in the [TransAT User Manual](#).

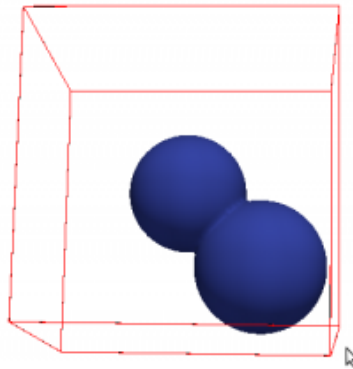


Figure 4: Interface between fluids created with user-defined initial conditions

## 2.3 Compressible multiphase flow model

The compressible model has been extended to multiphase flows.

### 2.3.1 Features

- Available equations of state
  1. Stiffened Gas
  2. Perfect Gas
  3. Tait Water
  4. Tait Ammonia
  5. Incompressible
- Automatically adjust system pressure - useful for cases where pressure keeps increasing
- Resolve pressure wave - for acoustics - time steps are based on velocity and sound speed
- Density of each phase can be output

**2.3.2 Boundary conditions**

- P0, T0 inflow BC for compressible homogeneous mixtures
- Inflow mass flow rate specification for single phase inlets
- Supersonic outflows can be treated

**2.3.3 Compatibility and restrictions**

- Pressure-based method
- Available for Interface tracking as well as Ensemble Averaged models
- Temperature equation has to be solved with Compressible flow
- Slip velocity model is not allowed with Compressible multiphase model
- LES for compressible flows is disabled
- Phase change for compressible 2-phase flows is not available

## 2.4 SArP convergence control module

The Smart Adaptive Run Parametrisation (SArP) module controls the convergence of simulations. It monitors solver convergence, residuals and time steps. Upon convergence issue detection in simulations, the correction and optimisation feature of the SArP module is automatically triggered to adjust the numerical parameters. Figure 5 and Figure 6 show examples of convergence improvements following adjustments of numerical parameters by the SArP module. In the two examples, the target residuals are not reached without the SArP module but they are reached in less than 2000 iterations with the SArP module activated.

Note that the SArP module does not handle parameter errors in physical models, boundary conditions or initial conditions. Its intended use is on pure numerical issues.

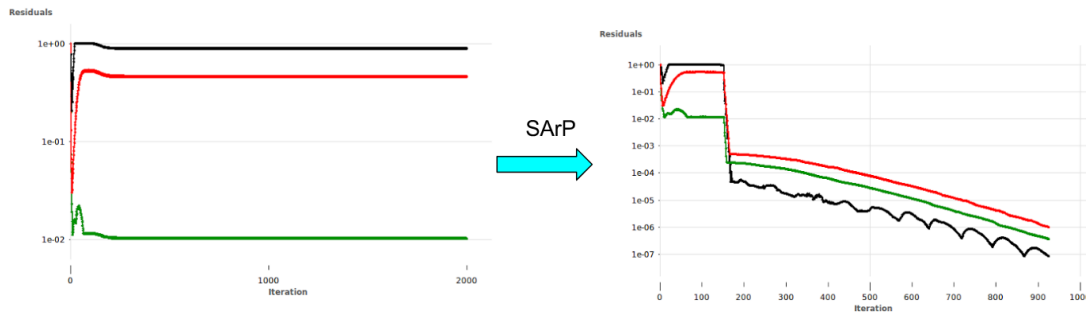


Figure 5: Example of correction with the SArP module (SArP module triggered after 150 iterations)

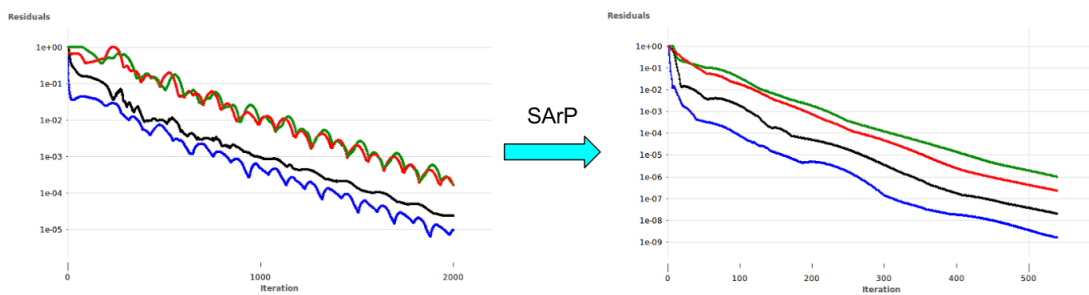


Figure 6: Example of optimisation with the SArP module (SArP module triggered at the beginning of the simulation)

## 3 Overview of the changes

### 3.1 Models

- Compressibility model extension for multiphase flows
- Sharp feature for immersed solids available as a beta feature
  - Full blocking effects of thin objects (compared to grid size) with only few grid points in solid
  - Full blocking effect for objects thinner than grid (no grid points inside solid)
  - Note wall shear is underestimated using this method, especially for thin objects
- RANS turbulence models
  - RNG (Renormalization Group Theory) k-epsilon high Reynolds model added

### 3.2 Graphical User Interface

- Display of Runtime Simulation Information in [TransATUI](#) during simulation run including:
  - Convergence and solver issues for each equation that is solved for
  - Residuals
  - Simulation messages (infos/warnings/errors)
- Automatic selection of primary variables solved for in Output Management window in [TransATUI](#)
- Addition of tab to set basic initial conditions

### 3.3 Simulation settings

#### Boundary Conditions

- New inflow options
  - Massflux option to define inflows
  - Addition of P0, T0 boundary conditions
- Definition of backflow conditions at outflows
- New option to define multiphase flow topologies at inflows

### Initial Conditions

- Addition of basic initial conditions which can directly be set in [TransATUI](#)
- Advanced initial conditions option using C++ solver interface

### 3.4 Post-processing

- Steady mass balance information
  - Writing of mass balance information for steady multiphase simulations
- C++ solver interface
  - Linear interpolation option added to the line output feature accessible in user defined functions
  - Addition of toolbox to performing basic parallel operations
  - Addition of entry points to access particle data
  - Addition of entry points to access wall boundary data (grid-level)
  - New options to extract heat flux, temperature, wall shear stress,  $y_+$  on wall boundary cells
- Automatic computation of reference lengths used for post-processing and non-dimensional numbers calculations
  - reference length is used in post-processing for non-dimensional numbers
  - automatic reference length computation based on domain and immersed solids
- Timesignal-Output
  - Setting of custom time signal points through a file
  - Writing of primary variables values for each time signal point
- Section-Output
  - Definition of custom section-planes through a file
  - Computation of integral quantities (volumes, mass-flux, etc.) on the section-plane/domain intersection

### 3.5 Windows Installation

- Installation workflow improvements
  - Check and installation of dependencies before TransAT installation
  - More flexible TransAT dependency detection (removal of hard-coded version detection)
  - Extra checks and operations added to alleviate common SDK 7 installation issues
- Improvement of installation error handling
  - Display of informative pop-up messages when errors occur or for any extra operation required to do after installation
  - Opening of files with troubleshooting instructions when common errors are detected
- Option to select Python executable to be associated with TransAT during execution (existing python installation satisfying requirements can be used).
- Simplification of default installer
  - Removal of ParaView from installer
  - Addition of an installer for Advanced Initial Conditions

### 3.6 Solver improvements and bugfixes

- Discretization improvements
  - pressure equation at fixed pressure boundaries reducing instabilities and therefore improving convergence
  - Close to immersed surfaces reducing instabilities significantly for large density ratio multiphase flows
- Fastmarching 1D/2D (used for domain wall distance calculation and LevelSet redistancing)
  - extension of the fastmarching algorithm to 1D/2D (until now only only 3D and 2D-xy planes were supported)
- Particle tracking
  - BMR grid support for particles
  - particle sub-stepping (when running simulations with time steps larger than particle cfl condition)

- particle restart from simulation without particle data
- Smooth time step adjustment close to the end of the simulation to match target simulated time. This prevents unphysical pressure gradient for incompressible flows due to the adjustment
- Inclined inflow
  - no inflow inclination allowed if volume- or mass-flow rate is defined
  - flow direction corresponds to the inflow bulk vector direction, even if inflow profile is applied
  - inflow flux remains equal to the flux defined by the boundary normal bulk velocity, even if applying an inflow profile
- Olga 7.2 Coupling
  - The client to run TransAT-OLGA coupled simulations via the OLGA built in OPC-Server has improved in stability, especially when running TransAT and OLGA on the same windows machine.
  - Two new command line options allow the user to display more information on the coupling communication in a new verbose mode and to store the whole console output in a separate log-file
- consistent variable output in tecplot/paraview format
- directory name error checking in [TransATUI](#)
- automatic windows/linux solid and input file conversion by [TransATUI](#)
- project directory permission error handling in [TransATUI](#)
- fix for scrollbars becoming inaccessible in the Execute Window of [TransATUI](#) after resizing the window