

## AthenaVisual Plus v21.1 to v22.0

1. **Fixed:** Miscellaneous bugs and cosmetic changes reported by the user community.
2. **Modified:** The implementation of the Runge-Kutta-Fehlberg integrator (RKPLUS) to be consisted with the DDAPLUS default integrator. The user now can switch from one integrator to the other, as long the system of differential equation has and  $E()$  Matrix equal to identity (i.e. System of Pure Differential Equations)
3. **Implemented:** The DIPPR 127H equation for the calculation of the ideal gas heat capacity.
4. **Modified:** All Physical property procedures to comply with the implementation of the new equation (DIPPR 127H) for the ideal gas heat capacity.
5. **Modified:** The integrator (DDAPLUS and RKPLUS) return logistics from a hard stop to a return to the calling program with additional information of the integration process up to the point of failure
6. **Fixed:** The calculation of the objective function during the line search when the user uses the prior information to update the model adjustable parameters for Bayesian Estimation.

## AthenaVisual Plus v21.1 to v21.2

7. **Fixed:** Miscellaneous bugs and cosmetic changes reported by the user community.
8. **Fixed:** Block Integration of experimental data with differential models that exhibit explicit discontinuities.
9. **Fixed:** Compilation bug when predictive mode in parameter estimation is enabled with Sensitivity Analysis option active.
10. **Implemented:** Parameter estimation graphics control pane with the responses displayed in a drop down list for easy selection. This feature is activated by setting **Param(152)=1**. The default value is **Param(152)=0**.
11. **Implemented:** Access to the Intel Fortran Compiler **oneAPI 2024**
12. **Implemented:** Code parallelization for parameter estimation with user explicit models when using the Least-Squares AthenaVisual Plus solver. This option is activated first by selecting **Allow for Code Parallelization** under **Tools: Preferences: Project Options** and then selecting **Enable Code Parallelization** in the Parameter Estimation Solver Control Panel: **Advanced Options**.
13. **Implemented:** Option to access the CPU Resource Monitor. This option is available under the **Tools** menu in AthenaVisual Plus.
14. **Implemented:** Option to enter the Intel Visual Fortran version via **Param(169)** and the Microsoft Visual Studio version via **Param(147)**. For instance the user may enter **Param(169)=2024.2** and **Param(147)=vs2022** or using the corresponding keywords **IntelFortranVersion=2024.2** and **VisualStudioVersion=vs2022**
15. **Fixed:** Model discrimination method based on the Akaike Information Criterion based on weights.
16. **Implemented:** Option to change the method for model discrimination and ranking based on the Akaike Information Criterion(AIC). The default method for discrimination and ranking is done based on **Weights**. There are two more methods one based on Akaike **Differences** and the other on the **Likelihood** of the candidate models.
17. **Implemented:** Option to enter the installation folder of Microsoft Visual Studio via **Param(124)**. For instance the user may enter **Param(124)=""C:\Program Files\Microsoft Visual Studio\2022\Community"**. The installation folder must be contained in quotes. When using this option the user must also enter the correct version of Microsoft Visual Studio using the keyword **VisualStudioVersion** as described above in item 8. The corresponding keyword for **Param(124)** is **VisualStudioFolder**
18. **Fixed:** Launching of the Microsoft Visual Studio for 64-Bit projects.
19. **Improved:** The PT Flash calculation has been improved for more robust convergence. Also upon failure it no longer throws a **Stop** command, rather it returns to the calling program with the value of  $v(ncc+8,10)=-1$  where  $v(ncc+8,10)$  is the final result of the flash calculation prior to failure.

## AthenaVisual Plus v20.0 to v21.1

1. **Fixed:** Miscellaneous bugs and cosmetic changes reported by the user community.
2. **Fixed:** The **Insert Function** menu item from the **Model** menu. Some external functions were misaligned in the list boxes. For each function now, the user can see the appropriate compiler in 32-Bit or 64-Bit mode
3. **Fixed:** Because of inappropriate default values of the **Param(121)** option, then number of bin for histogram plots was sometimes set to 1 and that cause AthenaVisual Plus to fail. This was fixed by setting the default value of **Param(121)** equal to 8: **Param(121)=8**
4. **Fixed:** Error capture when using Microsoft Visual(MS) Studio for the very first time and the association of **.sln** files to MS Studio was missing.
5. **Modified:** The IFORTvariables.bat file to accommodate oneAPI 2023
6. **Changed:** **Prt** keyword in Solver Options to **PrintLevel**.
7. **Implemented:** User can now specify the ASPEN Plus version using **Param(150)** and instruct AthenaVisual Plus to run a standalone model that calls ASPEN Plus Flash routines with **Param(151)**. The corresponding keywords are **AspenPlusVersion** and **AspenPlusRun**.
8. **Fixed:** A bug in the License manager that incorrectly processed user names.

## Athena Visual Studio v14.2 to AthenaVisual Plus v20.0

1. **Fixed:** Miscellaneous bugs and cosmetic changes reported by the user community.
2. **Overhauled:** The entire software package was overhauled to adhere to the new Windows Operating systems (10 and now 11) with numerous changes in the Graphical User Interface (GUI), the Fortran Compilers, the solvers for estimation and integration of ODEs and PDEs, and the Physical Properties methods that now include new equations of state, flash calculations as well as bubble point and dew point calculations. It is next to impossible to describe all the changes that went into effect with this overhaul of the software. Finally the software was modified in order to generate both 32-Bit and 64-Bit Dynamic Link Libraries for seamless interface with Microsoft Excel and Commercial simulators (ASPEN Plus, ASPEN Hysys and UniSim)

## Athena Visual Studio v14.1 to v14.2

1. **Fixed Bugs:** Miscellaneous bugs reported by the user community.
2. **New Feature:** Parameter **Param (205)** in the **@Solver Options** section if set to a value greater than zero forces Athena to stop at a discontinuity point other than the very first one. For instance setting Param (205)=1 will force Athena to stop at the second discontinuity point if it exists.
3. **License Information:** Updated Athena Visual Studio License information. To view the update from the **Tools** menu select **Athena Visual Studio License Manager** and then click **View Athena Visual Studio License Terms**.

## Athena Visual Studio v14.0 to v14.1

1. **Fixed Bugs:** Miscellaneous bugs reported by the user community.
2. **User Functions:** Added an option to use Fortran 90 syntax for user functions. In this way the user has the freedom to specify vector as well as complex functions. See Athena Visual Studio example in the ...\\Samples folder (**mcComplex.avw**).
3. **Keyword:** Added new keywords for solver control via the **@Solver Options** section in the modeling code. To view all keywords, open an Athena Visual Studio project and from the **View** menu select **Solver Parameters**.
4. **New Functions:** Added new functions *rand* and *randNormal* to generate random numbers from uniform and normal distributions. See Athena Visual Studio help file for details of the implementation of these functions and examples in the ...\\Samples folder (**mcRand.avw** and **mcMonteCarlo.avw**).
5. **New Functions:** Added new mathematical functions *FirstOrderDerivative* and *SecondOrderDerivative* and *FluxDerivative* to calculate derivatives using Finite Difference formulas on uniform grids. See Athena Visual Studio help file for details of the implementation of these functions and examples in the ...\\Samples folder (**mcFiniteDifferences.avw**).
6. **New Functions:** Added new physical property functions *EnthalpyForm* and *GibbsForm* and *StdLiqDensity* to calculate the standard enthalpy of formation, the standard Gibbs free energy of formation and the standard liquid density of user selected components. See Athena Visual Studio help file for details of the implementation of these functions and examples in the ...\\Samples folder (**mcPhysicalProperties.avw** and **mcPPHelp.avw**).
7. **New Feature:** Parameter **Param(204)** in the **@Solver Options** section if set to one forces Athena to use the Run Sequence Plot as the default. If it is set equal to zero forces Athena to use the Parity plot as the default.
8. **New Feature:** A submenu in the **Parameter Estimation Solver** control panel allows the user to select all responses for estimation and also to clear the selected responses. The submenu is activated by a right mouse click on the list box that displays all the responses.

## Athena Visual Studio v12.3 to v14.0

1. **Block Data Structure:** Beginning with v14.0 users will be able to define block data structures for parameter estimation from multiresponse data. See example **PEM25.avw** in the C:\Program Files\Athena\Samples\Parameter Estimation Models folder.
2. **New Functions:** Added new functions *Simpson* and *Gauss* for the calculation of the definite integral of smooth functions. See Athena Visual Studio help file for details of the implementation of these functions and examples in the ...\**Samples** folder (**mcFunIntegral.avw** and **mcSimpson.avw**)
3. **Fixed Bugs:** Miscellaneous bugs that were persistent in the VisualKinetics Module.
4. **Updated Chemical Engineering Topics Help:** Miscellaneous improvements to the Chemical Engineering subjects that are described in this help file.
5. **Plot Functions under Tools menu:** This option has been extended to include user models that can be supplied via Dynamic Link Libraries that can be generated by Athena Visual Studio. The names of these DLLs must be **Sub Fx(x,y,iFx)** for two-dimensional plots and **Sub Fxz(x,z,y,iFzx)** for three-dimensional plots. The integer arguments **iFx** and **iFzx** allow the user to enter more than one function in the same subroutine. Furthermore the following functions have also been implemented:

*min, max, range, sum, gamma, gami, gamic, psi, erf, erfi, erfc, erfci, beta, betai, ndist, ncdist, ninv, tdist, tcdist, tinv, fdist, fcdist, finv, chidist, chicdist, chiinv, wdist, wcdist, winv, lndist, lncdist, lninv, betadist, betacdist, betainv, gammadist, gammacdist, gammainv, besj, besy, besi, besk.*

All these functions are described in detail in the Athena Visual Studio Help file. The syntax for calling the user DLLs is  $y=F_{xz}(x,z,1); y1=F_{xz}(x,z,2)$ . These DLLs must be placed in a folder that is in a searchable by Windows path such as C:\Windows.

6. **Type Variables:** *Type* variables can now be coded in Athena Visual Studio as follows:

```
$$Type Input
$$ Real*8:: Temperature
$$ Real*8:: Pressure
$$ Real*8:: Composition(100)
$$ Real*8:: Kvalues(100)
$$End Type Input
```

```
Dim myInput As Type(Input)
Input%Temperature=200.0
```

A better way to implement *Type* variables is via a module. That gives the user more flexibility. An example of that can be found in the Athena Visual Studio samples folder \Athena\Samples\Fortran90\TestModule.avw

7. **New Subroutine:** A new subroutine has been added in the **AthenaUtilities** module. The subroutine **HessianMatrix( FCN, X, Hess [,Gradient] [,Eps] )** can be used to calculate the Hessian matrix and the Gradient vector of a scalar function that is supplied by the External FCN. An example of that can be found in the Athena Visual Studio samples folder **\Athena\Samples\Stand Alone Models\mcHess.avw**. This example is fully functional with the Compaq and Intel Visual Fortran Compilers. If you are using the g95 compiler you must delete the references to the **Athena** module and the call to **mcHess** subroutine and the **Hessian** function.
8. **Fixed Bug:** The **Help** command button was disabled in the **Fortran and Code Generation Options** menu item under **Build** for the Compaq and Intel Compilers. This bug was been fixed in v14.0
9. **Update Help File:** Updated the *Fortran Programming Review* section of the **Fortran Compilers Help** file.
10. **New Statement:** Implemented the *NameList* Fortran specification statement. The *NameList* statement specifies a list of variables which can be referred to by one name selected by the user, for the purpose of performing input and/or output. An example of this specification statement can be found in the Athena Visual Studio samples folder **\Athena\Samples\Ordinary Differential Equations\ODE20.avw**.
11. **Fixed Bug:** Sensitivity analysis with respect to initial values for differential and partial differential equations would not work if the number of equations was a variable and not a number. This bug has been fixed in v14.0.
12. **Fixed Bug:** A bug was fixed in the **Replace** text window in the Athena Editor. The bug would show only if there were blank lines at the end of the user code and the **Replace All** command was issued followed by the **Find Next** command.
13. **New Feature:** Added function **doubleIntegral** to calculate definite double integrals>. An example of this function can be found in the Athena Visual Studio samples folder **\Athena\Samples\Stand Alone Model\mcDoubleIntegral.avw**
14. **Update Help File:** Updated the *General Mathematics Module* section of the **Athena Visual Studio Help** file.
15. **New Feature:** Beginning with version v14.0 the user will be able to pass the Number of Equations, Number of Integration Points and Number of Continuation points as arguments into model subroutines for algebraic and differential models. This can be accomplished by issuing the following statement in the Solver Options section of the Athena code: **variableNEQ=myNeq;myNpts;myNptcon**. Here **myNeq** is the number of equations, **myNpts** the number of integration points and **myNptcon** the number of continuation points.
16. **New Feature:** Beginning with version v14.0 the user will be able to pass the Number of Equations, Number of Grid Points, Number of Break Points, Number of Integration Points and Number of Continuation points as arguments into model subroutines for partial differential and boundary value models. This can be accomplished by issuing the following statement in the Solver Options section of the Athena code: **variableNEQ=myNeq;myNgrid;myNbreak;myNpts;myNptcon**. Here **myNeq** is the number of equations, **myNgrid** the number of grid points per element, **myNbreak** the number of breakpoints, **myNpts** the number of integration points and **myNptcon** the number of continuation points

17. **New Feature:** Beginning with version v14.0 Athena will offer a number of functions to perform Flash calculations for Vapor/Liquid mixtures as well as Flash calculations of mixed streams with conventional components and solids. Please check the Physical Properties documentation for detailed information.
18. **New Feature:** Beginning with v14.0 Athena will offer two functions *pSteam* and *wSteam* that will calculate steam and wet steam properties. To view a description of these functions check the Physical Properties book under Athena Visual Studio Help.
19. **New Feature:** Beginning with version v14.0 Athena will offer a splines calculation block for easy interpolations. The block contains three functions: AkimaSplines, Cubic Splines and Quadratic Splines. Please read the General Mathematics Module help on Spline Interpolation.
20. **New Feature:** Beginning with version v14.0 the Runge-Kutta methods for the integration of mildly stiff ODE's have been enhanced to handle explicit discontinuities in the time domain.
21. **New Feature:** Beginning with version v14.0 users will be able to identify solid components in the Physical Properties window. Set the **Solid State** to 0 for a conventional component or 1 for a solid component.
22. **New Feature:** Beginning with v14.0 a new interface to the Athena functions and utilities has been implemented. The interface categorizes the functions into Fortran, Mathematical and Numerical, Statistical, Text and Utilities, Thermo and Unit Conversions so that it is very transparent to the user. The help files have also been updated to reflect the new architecture for the Athena Functions.
23. **New Feature:** Object files linked to the user project no longer need to be placed in folders with empty spaces in the path name. An API that converts long path names to short path names has been implemented, so that the path names are compatible and the command option of the Compaq and Intel Visual Fortran Compilers.
24. **New Feature:** Beginning with v14.0 users will be able to link the Athena Libraries with stand alone Fortran code.
25. **New Feature:** Beginning with v14.0 users will be able to use the **includeLocal** keyword to includes parts of Fortran compatible code anywhere in their Athena project. Furthermore the **\$include** keyword allows for the user to insert declaration statements that are coded in a separate file. The files accessed by the **include** and **includeLocal** keywords must have filetype **.for** or **.f**
26. **New Feature:** Beginning with v14.0 the user will be able to enter all the elements of the **Param( 1 to 200 )** vectors that controls the Athena solvers through the **@Solver Options** section. To view a brief description of all Param(1 to 200) elements, open Athena Visual Studio , and from the View menu select Solver Parameters.

27. **New Feature:** Beginning with version v14.0 users will be able to specify blocks of code as comments. The block of code is marked as follows:

```
!*BEGIN: Start block of code that will be commented out by the Athena parser
!-----
    Statement 1
    Statement 2
    :
!*END: End block of code that will be commented out by the Athena parser
!-----
```

**!\*BEGIN** and **!\*END** are required keywords. Anything else is optional. To request the Athena parser to process this block of code simply remove the **\*** character from the **!\*BEGIN** keyword.

## Athena Visual Studio v12.2 to v12.3

1. **Updated Parameter Estimation Tutorial:** Added description on the use of sensitivity analysis for the calculation of the gradient vector
2. **Updated Athena Visual Studio Help:** Updated the section on Parameter Estimation with Implicit Models to synchronize with the **Parameter Estimation Tutorial**.
3. **Updated General Mathematics Module:** Update the documentation of the General Mathematics Module and introduced a complete set of functions for the LQ Decomposition of a rectangular matrix  $A(m,n)$ . The old *getQ* function was replaced by the *getQ1* because it was calculating the  $Q_1$  and NOT the  $Q$  matrix of the LQ decomposition. The complete set of functions for the LQ Decomposition of a rectangular matrix with full row rank, is given in the Athena On Line Help manual. To access it, open **Athena Visual Studio** and from the **Help** menu select **Athena Visual Studio Help** and then click **General Mathematics Module**. From there, you may select the topics **Matrix Operations** and **Matrix Operations...Continued**
4. **Fixed Bug:** In the previous versions of Athena Visual Studio the semi-normalized sensitivity coefficients were computed incorrectly at the break points in the time-like dimension for mixed systems of differential and algebraic equations. The calculation was also incorrect for systems where the initial values of the first order sensitivity functions were non-zero. This bug has been fixed in version 12.3
5. **Updated Stand Alone Models Folder:** Updated and cleaned up the folder that contains User Defined Models (Stand Alone Models). All examples now have a suitable self-descriptive name.
6. **Minor Improvements:** In the Graph control panel textboxes the Fonts were changed to Arial and the 3D graphics in the solution of PDEs were improved.
7. **License Manager:** License manager was updated to accommodate users with very restricted privileges in University Networks. This feature applies only to Academic License holders.
8. **Update Athena Visual Studio Help File:** Updated the Miscellaneous Topics book in the Athena Visual Studio Help file to reflect the addition of new keywords for drawing true 3-dimensions graphs. The new keywords are Elevation, Rotation and Perspective.
9. **New Feature:** Introduced a new feature; under the **Tools** menu the user can select **Plot Functions** in order to plot 2-dimensional ( $y=f(x)$ ) and 3-dimensional functions ( $y=f(x,z)$ ).

## Athena Visual Studio v12.1 to v12.2

1. **Add Function:** Added the `char` Fortran Intrinsic in the reserved words list.
2. **Fix Bug:** Fixed a bug occurring when the user selected a compiler in the **Options** window. The g95 compiler tab was not disabled or enabled based on the user's selection.
3. **Fix Bug:** Fixed a bug occurring when setting up Parameter Estimation or Nonlinear Optimization problems from Process Models that are active in Athena. The setup is now canceled when user changes his/her mind or chooses the same file name for estimation/optimization as the one for the Process Model.
4. **Fix Bug:** Fixed a bug occurring when user double-clicks in an Error window (*myAPP.ERR*) to locate an offending statement when a floating point exception or FORTRAN compilation error occurs. There is no check to ensure that the offending line number does not exceed the number of lines in the file that contains the offending statement. This error was not trapped and it caused Athena Visual Studio v12.1 to close.
5. **Add New Example:** Added the Rat43 test case form the NIST Statistical Reference Datasets <http://www.itl.nist.gov/div898/strd/> in the installation folder C:\Program Files\Athena\Samples\NIST Statistics.
6. **Fix Bug:** Fixed a bug occurring when the user selects the compilation option `-fpe:0` (under the Compaq and Intel Visual Fortran Compilers). Athena's engine throws an exception due to overflow. This exception comes from the LAPACK function DLAMCH that computes machine parameters. This bug has been fixed via a keyword through the **Solver Options**. To avoid the floating point exception thrown by Athena's engines when the `-fpe:0` option is used, the users sets *MachineParameters*=1 in the **Solvers Options** section of the Athena code.
7. **Athena Interface:** Minor updates to the *Welcome: New Mode Selection Panel* Window
8. **Athena Interface:** Updated the Athena Toolbar by adding a button to online Help. Fixed small errors in the shortcuts of various menu items. Some items were given the same shortcut letter.
9. **Fix Bug:** Fixed a bug in the Partial Differential Equations training sample. The equation form based on the dimensionless state variables was incorrect.
10. **Fix Bug:** Fixed a bug in the Visual Kinetics Control Panel. Second option for the selection of the reaction rate constants did not update the headers of the corresponding spreadsheet
11. **Fix Bug:** Fixed a bug in the Optimal Experimental Design control panel. The data file with the proposed experimental design was very large because of the way it was saved. The file now is only a few KB large.
12. **Athena Tutorials:** Added a Nonlinear Optimization Tutorial
13. **Athena Tutorials:** Added a Boundary Value Problems Tutorial
14. **Athena Tutorials:** Added a Partial Differential Equations Tutorial
15. **Athena Tutorials:** Added a Visual Kinetics Tutorial

16. **Athena Sample Files:** Updated description of Athena Samples in the **Algebraic Models** folder, **Partial Differential Equations** folder and **Nonlinear Optimization** folder
17. **Athena Interface:** Enhanced Athena Toolbar with two shortcuts for debugging with Intel and Compaq compilers, and optimal experimental design
18. **Athena Training Samples:** Added a Nonlinear Constrained Optimization sample.
19. **Update Help Files:** Update the *Athena Knowledge Base* help file.
20. **Update Help Files:** Update the *Chemical Engineering Topics* help file
21. **Update Help Files:** Update the *Athena Visual Studio Help* file
22. **Update Help Files:** Update the *Fortran Compilers Help* file
23. **Update Help Files:** Update the *Athena Solvers Help* file

# Athena Visual Studio v11.0 to v12.1

## General Improvements

1. Introducing the Athena Visual Studio Knowledge Base
2. Ability for Version Control (Compaq and Intel Compilers only)
3. Enhanced Chemical Engineering Help Material
4. Enhanced Statistical Methods Help Material
5. Enhanced Tutorials for Beginners
6. On-Line Compiler Options
7. Numerous Mathematical and Statistical Functions
8. Detailed Documentation of Mathematical and Statistical Functions
9. Added Graph Configuration File
10. Added Component Insert Mode in Physical Properties
11. Ability to create DLLs with Variable Number of Equations
12. Ability to create Closed and Open Form Models with Variable Number of Equations
13. Ability for User to Enter FORTRAN 95 Variable Declarations
14. Seamless integration with the Compaq Visual Debugger with a Single Click
15. Seamless Integration with the Intel Visual Debugger with a Single Click
16. New License and Security Manager
17. 15 Day FREE Evaluation Period (extended to 30 Day upon request)
18. FREE Classroom Instruction License with Purchase of the Academic Research License
19. Athena Visual Studio v12.1 runs under Windows VISTA
20. User Account Control (UAC) Manager for Windows VISTA
21. Improved, Searchable and well Organized Documentation
22. Getting Started Help for Beginners
23. New Expanded and Improved Monitor Statement
24. Implementation of Shape-Preserving Quadratic Spline Interpolation
25. Improved Interfaces and Bug Fixes from User Feedback
26. Smart User Code for Solver Manipulation and Solver Options Command Section
27. Enhanced Printing (Jacobian Matrices) and Troubleshooting

## **Parameter Estimation and Model Discrimination**

1. Introducing Improved and Enhanced Optimal Experimental Design
2. Continuous Monitoring of the Estimation Progress (for Large Problems)
3. Simultaneous Integration of Blocks of Experimental Data for Fast Estimation
4. Version 12.1 Allows for Missing Settings and Responses
5. Version 12.1 Allows for Character Settings (ex. Catalyst Name or Type)
6. Version 12.1 Allows the User to Select Responses for Fitting
7. Grubbs' Test for Detecting Outliers

## **Ordinary Differential and Algebraic Systems**

1. State and Sensitivity Vector Relative and Absolute Tolerances
2. Implementation of Runge-Kutta 4th and 5th Order Integration Algorithms
3. Implementation of Explicit Auxiliary Variables
4. Introducing Ability to Store Integration History (Successful Steps)

## **Partial Differential Systems**

1. Setup the Framework for Two-Dimensional Partial Differential Equations
2. New Discretization Schemes for Hyperbolic PDEs
3. Inhomogeneous domains with state and flux discontinuities
4. State and Sensitivity Vector Relative and Absolute Tolerances
5. Finite Differences on Finite Elements with User Imposed Continuity Conditions
6. Implementation of Explicit Auxiliary Variables