USimQuickStart

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USIM QUICK START: GETTING STARTED WITH THE USIM SERIES OF COMPUTATIONAL APPLICATIONS

Welcome to the USim series of computational applications, *powered by the Ulixes computational engine*. Ulixes is a general purpose fluid plasma modeling code that supports shock capturing methods for MHD, Hall MHD, Two-Fluid plasma, Navier Stokes, and Maxwell's equations as well as multi-species, multi-temperature versions of the fluid systems mentioned. The equation systems can be solved on bodyfitted and unstructured grids in 1, 2, and 3 dimensions. Navier Stokes and MHD models allow for user specified equations of state along with the ability to use PROPACEOS tables (purchased from Prism Computational Sciences). USim has the ability to model the plasma device as part of a circuit. Recent applications of USim have included modeling merging plasma jets, laboratory accretion disk experiments, weakly ionized hypersonic flow modeling, magnetic nozzles and capillary discharges. USim is a multi-platform tool and runs on Windows, OS X, and Linux.

This manual, *USim Quick Start*, provides hands-on training for new users of the USim series of computational applications. It demonstrates how to carry out simulations using the USimComposer interface to the input files.

The USimComposer interface allows you to edit and validate your simulation input files, run simulations in either serial or parallel (thereby utilizing multiple cores or even computational nodes that do not share memory), and visualize results. USimComposer provides GUI editing of the main input variables of appropriately marked-up input files. However, one can still edit input files in any text editor, execute through the command line and visualize in any tool that understands the HDF5 output.

USim installation instructions are given in the document, installation.

The subsequent sections provide examples that can be run through USimComposer. Each section is named for the USim package or module that is needed to run those examples. That is, the USimBase chapter contains the examples that can be run with a USimBase license, for example. All examples can be run with a full USim license.

After learning how to run the USim applications through USimComposer, you can turn to the manual, usim-in-depth, to learn how to edit input files directly to create your own custom simulations. All input file blocks are specified in the manual, usim-reference.

CHAPTER

USIMCOMPOSER INTRODUCTION

This introduction to the USimComposer Graphical User Interface demonstrates setting up, running, and visualizing simulations. The rest of *USim Quick Start* assumes that you have reviewed this section to familiarize yourself with the USimComposer GUI.

The first sub-section provides an explanation of the basic workflow through the application - consisting of the three steps Setup, Run, and Visualize. Following this portion of the document is a detailed explanation of the options and commands available through the menu bar at the top of the USimComposer window. Finally, this section includes explanations of the default USim settings supplied by USimComposer.

In the HTML version of this document, click on any illustration to see a full size view. The images presented in this section have been captured on a computer running Mac OS X; the USimComposer interface will appear slightly different on Windows and Linux platforms.

Setup Window showing main USimComposer parts. illustrates the layout of the USimComposer GUI using labels for the parts of the interface to which this introduction and the tutorials refer.

2.1 Setup

2.1.1 Create New Runspace From Example

To run one of the examples in USim, one must first create a runspace from the many templates that come with USim. There are two ways to create a runspace from one of the templates. The first is to choose "New from Template..." from the File menu. The second is in the **Setup Window**. In the **Setup Window**, click on the **New** button next to *New From Template...* in the middle of the **Setup Window**.

2.1.2 Select Example Template

From the "New from Template" dialog, choose a new example template from one of the packages. Only those templates which you have licensed will run, though all examples will still be shown.

If you have clicked once on your selection in the *Choose Example* pane, your selection is highlighted. Now click on the **Choose** button in the lower right area of the **New from Template** window as in *Selecting an example from the "New from Template" Dialog*. Alternatively, you could double-click on an example name and USim will behave the same as if you had selected the example and then the **Choose** button.

For this example we will use the "USimBase - Flow over a forward facing step" example.



Fig. 2.1: Setup Window showing main USimComposer parts.

000	U USimComposer
U	
Welcome	
2	
Setup	Setup Window
Run	No runspace open. Please try one of the following:
Visualize	New from Template New
Help	Open Runspace Open

Fig. 2.2: Setup Window



Fig. 2.3: Selecting an example from the "New from Template" Dialog

2.1.3 Choose a Name for the New Runspace

The window **Choose a name for the new Runspace** allows you to choose the directory to which the example files will be copied from the template. The default name of the directory is displayed in the *FileName* field. For this example, the default name is forwardFacingStep. If you want to use a different name, you may type a different name into the *FileName* field. When you are satisfied with the directory name and location, click the **Save** button to proceed.

Use Smart Grouping	, bocuments,		15	
▼ filename	size	last accessed		
🛛 🚳 [parent directo	ory]			
🕨 🥥 anisotropicDiffu	sion	10/22/13 15:44:48.000		
🕨 💭 brioWu		10/18/13 10:06:24.000		
🕨 💭 brioWu1		10/22/13 15:42:53.000		
brioWu2		10/24/13 21:26:20.000		
🕨 💭 brioWu3		10/29/13 12:17:31.000		
🕨 💭 brioWu_dave		11/25/13 12:24:05.000		
🕨 💭 brioWuPar		10/23/13 14:08:20.000		
🕨 🥥 collisionalMultiF	luid	10/21/13 12:02:09.000		
ilter by: All Files				÷
Name: forwardEacing	Sten			
Name: forwardFacing	Step			

Fig. 2.4: Create Directory to Use for Runspace

2.1.4 Using the Setup Window

After you choose the name for the runspace, USimComposer displays the **Setup Window** containing a *Navigation* pane on the left and an *Editor* pane on the right. The workflow panel remains available on the far left.

Below the *Runspace Files* tab in the *Navigation* pane you will find a pulldown menu for which files are shown, which defaults to *All Files* and a toggle choice of *Smart Grouping*, which is on by default. These menus determine the format in which files will be displayed in the Files tab. Depending on how complex a simulation is, there may be multiple files used in a simulation, including the input file, macros, and python geometry files. Many more files produced during the simulation run at each time step of the run.

To enable convenient viewing of the list of simulation files, USim allows you to specify in what order as well as which type(s) of files you would like to view. *Smart Grouping* causes similar types of files to be displayed in the same area of the Files tab list. Turning off *Smart Grouping* causes files to be displayed in alphabetical order rather than by type. *All*

00		USimComposer – forwardFacingStep.pre
	Navigation	Editor
Welcome	Runspace Files /Users/alexanda/Document s/txcorp/USimComposer2.0 /runs/forwardFacingStep	Image: Save And Process Setup Image: Setup Ima
Run Visualize	filename forwardFacingStep forwardFacingStep.in forwardFacingStep.pro forwardFacingStep.pre forwardFacingStep1.m	CFL 0.4 T_FINAL 4.0 N_FRAME 20 Compressible inviscid flow over a step using on an unstructured mesh
Help	 forwardFacingStep2.m forwardFacingStep_0.l forwardFacingStepGrid forwardFacingStepTn.p forwardFacingStepVars ntMesh.msh 	MESH_FILE facingStep1.msh" RIEMANN_SOLVER "hlleFlux" VARIABLE_FORM "conservative" LIMITER "muscl" GAMMA 1.4
	All Files Smart Grouping Refresh Open	

Fig. 2.5: Setup Files Tab

Files indicates that you want to see all available files involved in the simulation. You could choose to limit your view to only *Runspace Files*, which are files such as input files and macros that can be edited in the USimComposer Editor pane, or *Text* files, which include all types of human-readable file formats, or *Data* files, which include incremental dump files and output files that can be visualized.

File name filtering with these pull-down menus is illustrated later in this document in the Visualization Pane section, *Results Pane*.

In addition to Runspace Files, the *Setup Window* holds the tab to change the key parameters for a run and the *Save and Process Setup* button. See *The main parts of the Setup Window*.

000	USimComposer - forwardFacingStep.pre
Navigation	Editor
Runspace Files	🐼 🗞 🛅 🐌 View Input File 🔬 Save And Process Setup
Velcome /Users/alexanda/Document s/txcorp/USimComposer2.0 /runs/forwardFacingStep	★ forwardFacingStep.pre
filename	CFL 0.4 "Save And Proce
Run i forwardFacingStep.in forwardFacingStep.in	T_FINAL 4.0 Setup" Button
forwardFacingStep.pre	N_FRAME 20
Help	MESH_FILE FacingStep1.msh*
forwardFacingStepOnt	RIEMANN_SOLVER "hileFlux"
ntMesh.msh	VARIABLE_FORM "conservative"
Runspace	LIMITER musci
Filos	GAMMA 1.4
Files	
	Key Input
All Files \$	Parameters
🔁 Refresh 📄 Open	

Fig. 2.6: The main parts of the Setup Window

Click on the **Save and Process Setup** button in the upper right corner of the USimComposer **Setup** window to validate the input before running USim.

2.1.5 Key Input Parameters in the Setup Window

All the example files in USimComposer come with key parameters allowing the user to easily adjust basic parameters of the simulation. The default setup window will show the key input parameters interface and an image of what the simulation looks like. By holding the mouse over the key input parameter title, a description of what exactly the

variable does will pop up. Many examples can actually be significantly modified with just the key input parameters and extended for slightly different applications.

000	USimComposer - forwardFacingStep.pre
Walgation Welcome Image: Setup Setup Image: Se	Editor View Input File Save And Process Setup Conversed Save And Process Setup Conversed Save And Process Setup Save And Process Setup Save And Process Setup Inviscid flow over a Step using on an unstructured mesh N_FRAME 20 MESH_FILE facingStep1.msh* RIEMANN_SOLVER "hlleFlux" VARIABLE_FORM "conservative" LIMITEB factorset GAMMA 1.4 Adiabatic index, or ratio of specific heats
All Files Smart Grouping Refresh Open	Key Input Parameter Mouse-Over Description

Fig. 2.7: Key input parameters or the full input file can be edited in the Setup Window

If you would like to see the actual input file, simply click on the *View Input File* in the upper left hand side of the *Editor* pane. This will bring you to the traditional .pre file.

2.1.6 Save and Process the Input File

Click on the **Save and Process Setup** button in the upper right corner of the USimComposer **Setup** window as illustrated in the image below.

2.1.7 View the Output Messages

USim notifies you of the actions that it is taking in a new window that USimComposer opens in the lower portion of the **Editor** pane.

Notice that this new window contains three tabs: a **Find/Replace** tab an **Output** tab and a **Results** tab. If you had clicked in any tab of the Editor window, the **Find/Replace** tab would have appeared to assist you with editing the file.

00		USimComposer – forwardFacingStep.pre	
U Welcome	Navigation Runspace Files	Editor Image: Solution of the second seco	A Save And Process Setup
Setup	/Users/alexanda/Document s/txcorp/USimComposer2.0 /runs/forwardFacingStep	× forwardFaci	ngStep.pre
Run	filename forwardFacingStep forwardFacingStep.in forwardFacingStep.png forwardFacingStep.png	CFL 0.4 T_FINAL 4.0	step using on an unstructured mesh
Visualize	 forwardFacingStep.pre forwardFacingStep1.m forwardFacingStep2.m forwardFacingStep_0.l 	N_FRAME 20 MESH_FILE =acingStep1.msh"	
	 forwardFacingStepGrid forwardFacingStepTn.r forwardFacingStepVars ntMesh.msh 	RIEMANN_SOLVER "hileFlux"	
		LIMITER "muscl"	
		GAMMA 1.4	
	All Files ‡		
	Smart Grouping		
		J	

Fig. 2.8: Save and Process Setup Button

The **Output** tab notifies you each step of the way as to what USim is doing as illustrated in *Setup Window tab for output message*.

S Find/Replace Output Results
Starting runspace setup. Creating input file. Processing file: /Users/alexanda/Documents/txcorp/USimComposer2.0/runs/forwardFacingStep/forwardFacingStep Preprocessing completed successfully. Proceed to run window.

Fig. 2.9: Setup Window tab for output message

2.2 Run

2.2.1 Select the Run Window

When your Save and Process activity completes successfully, USim reminds you that you can now proceed to the run part of the workflow. To do this, click on the *Run* button in the workflow panel on the far left of the USimComposer window (see *Setup Window showing main USimComposer parts.*).

2.2.2 Using the Run Window

As in the USimComposer Setup window, the USimComposer Run window contains two panes. As displayed in *Run Window Figure*, the **Runtime Options** window on the left contains a **Standard** tab and a **MPI** tab. The Logs and Output Files pane on the right contains a **Engine Log** tab on the left and a **File Browser** tab on the right.

2.2.3 MPI (Parallel Execution) Options

USimComposer runs simulations in serial by default. If you are running on a local system with multiple cores, you can run your simulation in parallel as multiple processes. The simplest method to tell USimComposer to run simulations in parallel is to switch the number of processors to run in the Run window. In the upper-right portion of the **Runtime Options** pane, there is a tab **MPI**. Here you can define the number to as few or many processes you want to run. If the Run with MPI button is unchecked the simulation will run in serial mode. See *Host Settings* for a description of how to set USim to run in parallel by default.

2.2.4 View the File Browser Tab in the Logs and Output Files Pane

In the previous step the **File Browser** tab was located behind the **Engine Log** tab in the **Logs and Output Files** pane. Click on the **File Browser** tab to bring it to the front as shown in *File Browser Tab in Logs and Output Files Pane*.

Notice that as with the **File Browser** in the **Setup** window, the **File Browser** in the **Run** window also has the *Smart Grouping* and *All Files* pull-down menus at the bottom of the tab.



Fig. 2.10: Run Window Figure



Fig. 2.11: MPI Options



Fig. 2.12: File Browser Tab in Logs and Output Files Pane

2.2.5 Run the Simulation

For our example, we'll run this simulation using only the default existing settings from the input file.

You do not need to select any file in particular in the **File Browser** tab before clicking on the **Run** button. However, if the **File Browser** tab display area is too narrow for you to see the full file names in the filename list and you would like to see the file name extensions of the files in the file browser, you can adjust the width of the filename field by using your mouse.

Click on the Run button at the top of the Logs and Output Files pane as shown in Run Button.



Fig. 2.13: Run Button

2.2.6 Stopping the Simulation

USimComposer features the ability to Force Stop a simulation. The button for this action is located next to the *Run* button (see *Run Button*).

If a Force Stop is used the field and history data will *NOT* be written to a .h5 file before the simulation stops. The output of a successfully force stopped simulation is given below.

	Runtime Options	Logs and Output Files
11	Standard MPI	Run Force Stor
Velcome	CAUTION: Overrides Existing Values	
F .		Engine Log File Browser
Satur	Restart at Dump Number	Component fluids: Taking step 20 from time = 0.235748 with dt = 0.00188149
Setup		Component fluids: Taking step 21 from time = 0.23763 with dt = 0.00188149
		Component fluids: Taking step 22 from time = 0.239511 with dt = 0.00188149
Run		Component fluids: Taking step 23 from time = 0.241393 with dt = 0.00188149
		Component fluids: Taking step 24 from time = 0.245274 with dt = 0.00188149
		Component fluids: Taking step 25 from time = 0.247037 with dt = 0.00188149
isualize		Component fluids: Taking step 27 from time = 0.248919 with dt = 0.00188149
		Component fluids: Taking step 28 from time = 0.2508 with dt = 0.00188149
<u> </u>		Component fluids: Taking step 29 from time = 0.252682 with dt = 0.00188149
негр		Component fluids: Taking step 30 from time = 0.254563 with dt = 0.00188149
		Component fluids: Taking step 31 from time = 0.256445 with dt = 0.00188149
		Component fluids: Taking step 32 from time = 0.258326 with dt = 0.00188149
		Component fluids: Taking step 33 from time = 0.260208 with dt = 0.00188149
		Component fluids: Taking step 34 from time = 0.262089 with dt = 0.00188149
		Component fluids: Taking step 35 from time = 0.265852 with dt = 0.00188149
		Component fluids: Taking step 37 from time = 0.267734 with dt = 0.00188149
		Component fluids: Taking step 38 from time = 0.269615 with dt = 0.00188149
		Component fluids: Taking step 39 from time = 0.271497 with dt = 0.00188149
		Component fluids: Taking step 40 from time = 0.273378 with dt = 0.00188149
		Component fluids: Taking step 41 from time = 0.275259 with dt = 0.00188149
		Component fluids: Taking step 42 from time = 0.277141 with dt = 0.00188149
		Component fluids: Taking step 43 from time = 0.279022 with dt = 0.00188149
		Component fluids: Taking step 44 from time = 0.280904 with dt = 0.00188149
		Component fluids: Taking step 45 from time = 0.282785 with dt = 0.00188149
		Component fluids: Taking step 46 from time = 0.284667 with dt = 0.00188149
	Reset Options	Engine completed with error: Process was stopped at user request.
_		

Fig. 2.14: Force Stopped Simulation

2.2.7 Restarting a Simulation

With USimComposer it is possible to restart a simulation that has been paused, or ended. This is useful if it is desired to add more time steps to the initial simulation, or if the simulation had been stopped in the middle of the run. Underneath the *Standard* tab of the *Runtime Options* pane of the run window there is a *Restart at Dump Number* field. Simply put in the last memory dump of the simulation and click on the *Run* button, like running a normal simulation. This process is demonstrated in the figure below.



Fig. 2.15: Restarting a Simulation

2.2.8 View the Engine Log

Just as when processing the setup, USim again notifies you of the progress of its activity by reporting results along the way in the **Engine Log** tab as shown in *Engine Log*. If the tab display area is full, scroll down to the bottom of the tab.



Fig. 2.16: Engine Log

2.3 Visualize

2.3.1 Selecting the Visualize Window

Notice that upon successful completion of the simulation run, the last message in the **Engine Log** tab is a reminder that you can now select the **Visualize** button from the workflow panel on the far left of the USimComposer window as seen in *Engine Log*. Remember that you may need to scroll down the *Engine Log* tab to see the completion message.

2.3.2 Visualize the Current Runspace Data

The simulation was successful and the next step is to visualize the data, Click on the **Open Button** in the **Visualize Window**.





2.3.3 Data Visualization Window

USimComposer's Visualization feature is a flexible and comprehensive model viewer based on VisIt. The simulation tutorials and examples in *USim Quick Start* provide several examples of using the Visualization feature's options in context.

The Visualization window is divided into a **Controls** pane on the left and a **Results** pane on the right.

As displayed in *Controls and Results Visualization Panes*, click on the right-facing triangle arrowhead next to **Scalar Data** and **Geometries** to expand the views.



Fig. 2.18: Controls and Results Visualization Panes

2.3.4 Controls Pane

By default, the Controls Pane will open **Data Overview** as the Data View. Other Data Views such as **Field Analysis** can be selected as shown in *Data View Menu*.



Fig. 2.19: Data View Menu

Variables

The *Variables* section of the **Controls** pane enables you to choose which aspects of the simulation data to visualize. The types of variables that are available in the *Variables* section are dependent on your particular simulation. Below are some typically available types of variables.

Scalar Data

Types of Scalar Data include:

- fluids/machNumber
- fluids/q_n



Fig. 2.20: Scalar Data Variables

Note that q_0 is mass density, q_1 , q_2 , and q_3 are the three components of momentum density, and q_4 is energy density.

Geometries

Types of Geometries include:

• fluids/domain

• fluids/domain_surface



Fig. 2.21: Geometries Variables

Contours (2-30)

The default value in the *Contours* field is 10. If you select the Display Contours check box and have an approriate data set selected the number of countours can be changed from 2-30

Log Scale Color Checkbox

If the appropriate field is selected the *Log Scale Color* checkbox will be available to enable and disable display of log scale color.

Annotation Level Menu

Use the Annotation Level pulldown menu to add or remove annotation from the visualization.

- No annotations
- Axes only
- Axes & Legends



Fig. 2.22: Contours



Fig. 2.23: Log Scale Color Checkbox

• All annotations



Fig. 2.24: Annotation Level

Reload Data

You can visualize data from a simulation run as soon as it becomes available in the runspace. If you decide to visualize data before a run is complete by switching to the Visualization tool and using the *Open visualization from current runspace* button in the Visualization window, USim continues creating data files in the background. Later when more data is available for visualization or the simulation run is complete, use the **Reload Data** button to visualize the new data.

Note: If the first visualization took place when there was only one dump, then the visualization system is completely reloaded, which means that plots are not preserved. However, if the first visualization took place when there was more than one dump, then all current plots and views are available when **Reload Data** is invoked.

2.3.5 Results Pane

The USimComposer Visualization Tool uses a window in the **Visualization Results** pane on the right side of the USimComposer window to dynamically display data modeled according to the selected variables and other **Controls** pane visualization configuration settings.

000	U	USimComposer	- forwar	dFacingStep	.pre			
	CONTROLS	VISUALIZATIO	N					
U	Data View: Data Overview +	2d						
Welcome	Variables	Save Image	Labels	Rendering	Colors	Reset View		
Setup Run Visualize	 Scalar Data Geometries 							
	Display Contours							
	Annotation Level: Axes & Leoond	Dump: 8	1 1	Ste	p: 878	1 1 1	Time: 1.6	· · · · ·
	Reload Data	0						20

Fig. 2.25: Controls Pane Buttons

Example Visualizations

The following images illustrate how the various features of the Visualization Tool can be used to control rendering of simulation data to help the user visually explore aspects of the simulation. Notice that the Visualization pane slider is used to adjust values for:

- Dump
- Step
- Time





Visualize Data from a Previous Run

In addition to visualizing the result of a current run immediately after conducting the simulation, you can also visualize data from a previous run. You can access recent simulations using **Recent Runspaces** in the **File** menu in the menu bar or the **Welcome** or you can locate all previous simulations using the *Open Existing Runspaces* in the *Setup Window*.

Open Recent Runspace from the File Menu

To access data to visualize from a recently conducted simulation, from the **File** menu in the menu bar, select **Recent Runspaces**.

File Edit Window Help		
📄 New from Template	U US	SimComposer – forwardFacingStep.pre
🎒 New from Existing		VISUALIZATION
ジ Open Runspace 第0 Open File in Editor	rview ‡	2d
Close Runspace Close File #W Close All Files	hNumber	Save Image Labels Rendering Colors Reset View
 J Save File 米S Save Image As J Save All 企業S 		Perudac der Vor nutling_1 - 8.081 - 5.902
Recent Runspaces 🔹 🕨	/Users/angle/Docu	ments/txcorp/USimComposer1.0/runs/forwardFacingStep/forwardFacingStep.pre
Help	Clear Recent Runs	0.000 Max: 11.40 Mr 0.000

Fig. 2.27: Recent Runspaces Selection in File Menu

Click on the name of the runspace whose data you want to visualize. USimComposer lists the existing data files in the selected runspace. Click on the **Yes** button if these are the files you want to visualize.

If you would prefer that USimComposer does not first list the names of the detected data files for you to inspect before deciding whether you would like to visualize that data, click in the checkbox labeled *Do not ask again*. Clicking in this checkbox will cause USimComposer from now on to immediately visualize the data from the selected runspace.

Open Runspace from the File Menu

If the simulation data you want to visualize was not produced recently, you can access the data from the **File** menu in the menu bar, select **Open Runspace...**.

Open an Existing Runspace from the Setup Window

Alternatively, if the simulation data you want to visualize was not produced recently, use the *Setup Window* instead of **Recent Runspaces**. Return to the **Setup** window by clicking on the *Setup* icon in the icon panel then select the **Open** button next to *Open Existing Runspace* as shown in *Existing Run Space button*.

USimComposer displays runspaces from which you may select.

If you did not previously elect not to display detected data files then just as with *Open Recent Runspace from the File Menu*, USimComposer displays a list of data files that it has detected in the selected runspace, and you can click on the **Yes** button to visualize the data.

Sorting and Filtering File List Display in the USimComposer File Browser

USim produces several different types of files with each simulation run. To make it easier to examine the files in a runspace, USimComposer provides the ability to sort the file list by file type or file name and to isolate particular kinds of files.



Fig. 2.28: Data Files Detected in a Runspace



Fig. 2.29: Existing Run Space button

⊖ ○ O U Open Runspace						
Host: localhost \$						
Path:	/Users/alexanda/Docu	ments/	txcorp/USimComposer2.0/runs			
📃 Use	Smart Grouping					
_		1				
	filename	size	last accessed			
	[parent directory]		10/22/12 15 44 40 000			
	anisotropicDiffusion		10/22/13 15:44:48.000			
	brioWu		10/18/13 10:06:24.000			
	brioWul		10/22/13 15:42:53.000			
	brioWu2		10/24/13 21:26:20.000			
	brioWu3		10/29/13 12:17:31.000			
	brioWu_dave		11/25/13 12:24:05.000			
	brioWuPar		10/23/13 14:08:20.000			
	collisionalMultiFluid		10/21/13 12:02:09.000			
	collisionalMultiFluid1		10/22/13 15:45:01.000			
	densePlasmaFocus		10/22/13 15:45:20.000			
Filter b	v: Runspace Files			\$		
				Cancel Open		
				open		

Fig. 2.30: Existing Run Space Selection
Sorting Files into Groups

The checkbox at the bottom of the USimComposer File Browser enables you to choose whether or not to sort the the list of files in a runspace. **Smart Grouping**, which is on by default, causes the type of files selected in the adjacent file type pulldown menu to be listed together in logical groups. If not selected, the type of files selected in the adjacent file type pulldown menu to be displayed in alphabetical order.

000	U	USimComposer – forwardFacingStep.pre	
	Navigation	Editor	
Welcome	Runspace Files	🔗 📦 📋 🍓 View Input File	A Save And Process Setup
Setup	/Users/angle/Documents/txcorp/USim Composer1.0/runs/forwardFacingStep	× forwardFacin	igStep.pre
Run	Image: size size Image: size Image: size Image: size	CFL 0.4	Compressible inviscid flow over a step using on an unstructured mesh
Visualize	forwardFacingStep.png forwardFacingStep.pre Kb forwardFacingStep.pre Kb forwardFacingStep.pre forwardFacingStep1 forwardFacingStep2 forwardFacing	T_FINAL 4.0	
	forwardFacingStep2.msh 457K	N_FRAME 20	
	 forwardFacingStepGrid.h5 65Kb forwardFacingStepVars.py 780b ntMesh.msh 101K 	RIEMANN_SOLVER "hileFlux"	
		VARIABLE_FORM "conservative"	
		LIMITER "muscl"	
		GAMMA 1.4	
	All Files \$		
	Smart Grouping		

Fig. 2.31: Smart Grouping of All Files

Filtering Files by File Type

The pulldown menu at the bottom of the USimComposer File Browser enables you to filter the display of files by file type.

All Files, which is the default, causes all file names to be displayed in the grouping indicated by the selected grouping method in the adjacent pulldown menu.

Data Files with Smart Grouping displays the folder containing data files in the runspace.

Data Files with Smart Grouping

Data Files with No Grouping displays the names of the data files inside the data file folder.

Other options are Text Files and Runspace Files.

000	U	USimComposer – forwardFacingStep.pre
	Navigation	Editor
Welcome	Runspace Files	🔊 🔊 👔 🌛 View Input File 🍐 Save And Process Setup
Setup	/Users/angle/Documents/txcorp/USim Composer1.0/runs/forwardFacingStep	× forwardFacingStep.pre
Run	filename size forwardFacingStep.in 41 forwardFacingStep.ng 17	CFL 0.4 Compressible inviscid flow over a step using on an unstructured mesh
Visualiza	forwardFacingStep.pre 7Kl	T_FINAL 4.0
	forwardFacingStep2.msh 45: forwardFacingStep_0.h5 75i forwardFacingStep_0.log 16f	N_FRAME 20
Help	forwardFacingStep_1.h5 75}	MESH_FILE indFacingStep1.msh"
	forwardFacingStep_11.h5 75 forwardFacingStep_12.h5 75 forwardFacingStep_13.h5 75 forwardFacingStep_13.h5 75	VARIARI E FORM "conservative"
	forwardFacingStep_15.h5 75	LIMITER "musci"
	 forwardFacingStep_16.h5 forwardFacingStep_17.h5 forwardFacingStep_18.h5 forwardFacingStep_19.h5 forwardFacingStep_19.h5 	GAMMA 1.4
	a forwardFacingStep_2.h5 751 a forwardFacingStep_20.h5 751 a forwardFacingStep_3.h5 751 a forwardFacingStep_4.h5 751	
/	All Files	
	Smart Grouping	

Fig. 2.32: No Grouping of All Files



000	U	USimComposer – forwardFacingStep.pre	
	Navigation	Editor	
Welcome	Runspace Files	🔗 🔞 😭 🌛 View Input File	A Save And Process Setup
	Composer1.0/runs/forwardFacingStep	s forwardFa	cingStep.pre
Run	 ▼ filename size forwardFacingStep_0.h5 75Kb d forwardFacingStep_1.h5 75Kb 	CFL 0.4	Compressible inviscid flow over a step using on an unstructured mesh
	forwardFacingStep_10.h5 75Kb forwardFacingStep_11.h5 75Kb	T_FINAL 4.0	
Visualize	 forwardFacingStep_12.h5 forwardFacingStep_13.h5 75Kb 	N_FRAME 20	
Help	forwardFacingStep_14.h5 75Kb forwardFacingStep_15.h5 75Kb	MESH_FILE IrdFacingStep1.msh"	
	 forwardFacingStep_16.h5 forwardFacingStep_17.h5 75Kb 	RIEMANN_SOLVER "hlleFlux"	
	forwardFacingStep_18.h5 75Kb forwardFacingStep_19.h5 75Kb	VARIABLE_FORM "conservative"	
	forwardFacingStep_2.h5 75Kb	LIMITER "muscl"	
	 forwardFacingStep_5.h5 forwardFacingStep_4.h5 75Kb forwardFacingStep_5.h5 75Kb forwardFacingStep_6.h5 75Kb forwardFacingStep_7.h5 	GAMMA 1.4	
	forwardFacingStep_8.h5 75Kb forwardFacingStep_9.h5 75Kb		
	forwardFacingStepGrid.h5 65Kb		
	Data Files +		
	Open		

Fig. 2.33: Data files with No Grouping

2.4 USimComposer Menu Bar

This introduction to the USimComposer menu bar presents features accessible from the menu bar.

2.4.1 Menu Bar

The USimComposer menu bar is located across the top of the USimComposer window.



Fig. 2.34: USimComposer menu bar

2.4.2 File Menu

The *File* menu contains options to control creating, opening, closing, and saving USimComposer files and runspace directories.

The New from Template feature is accessed from the USimComposer File menu.

Categories of templates from which to choose are listed in the left **Available Templates** pane of the **New from Template** window. The description of the selected category is displayed in the right **Description** pane of the **New from Template** window.



Fig. 2.35: File Menu



Fig. 2.36: New from Template Menu Selection

The *USimBase* category contains a number of example simulation files that are used in *USim Quick Start* and available with any USim license. As with the example categories, names of examples are listed in the left **Available Templates Example** pane with the description corresponding to the currently selected example shown in the right **Description** pane.

Available Templates Description V USimBase: Examples demonstrating the basic Brio & Wu Shock Tube Flow over a forward facing step Kelvin Helmholtz Instability MHD Ramp Flow Rayleigh Taylor Instability Sod Shock Tube Unstable plasma z-pinch These examples show how to study basic physics problems in USim. All of these can be executed with only a USimBase license. • USimHEDP: Examples demonstrating high en • USimHES: Examples demonstrating multifluid	000	Vew from Template
	Available Templates VUSimBase: Examples demonstrating the Brio & Wu Shock Tube Flow over a forward facing step Kelvin Helmholtz Instability MHD Ramp Flow Rayleigh Taylor Instability Sod Shock Tube Unstable plasma z-pinch USimHEDP: Examples demonstrating hig USimHS: Examples demonstrating multiplated VSimHS: Examples d	New from Template Description basic These examples show how to study basic physics problems in USim. All of these can be executed with only a USimBase license. th en fluid
Choose Cancel	USimHS: Examples demonstrating multing mult	fluid

Fig. 2.37: USimBase Example list

To open a runspace directory where existing simulation files reside, select **Open Runspace** from the **File** menu.

The runs directory in the USimComposerX.X directory that is created in your home directory when you install is the default directory in which runspace directories will be created when you use USimComposer to set up simulations.

2.4.3 Edit Menu

The Edit menu contains commands that pertain to editing activities in the Editor pane of the USimComposer window during Setup.

2.4.4 Preferences or Tools Menu

The **Preferences** (Mac OS X) or **Tools** (Linux/Windows) menu provides access to global settings for USimComposer applications from the icon panel.

Select USimComposer -> Preferences (Tools -> Settings) to access the Application Settings window.

The Applications Settings window is displayed with General highlighted.



Fig. 2.38: Open Runspace selection from File menu

00			U Open Runspace	
Host:	localhost		\$	
Path:	/Users/alexanda/Docu	ments/	txcorp/USimComposer2.0/runs	
🗌 Use	Smart Grouping			
•	filename	size	last accessed	1
6	[parent directory]			
🕨 🌔	anisotropicDiffusion		10/22/13 15:44:48.000	
🕨 🌔	brioWu		10/18/13 10:06:24.000	
🕨 🌔	brioWu1		10/22/13 15:42:53.000	
🕨 🌔	brioWu2		10/24/13 21:26:20.000	
🕨 🌔	brioWu3		10/29/13 12:17:31.000	
🕨 🌔	brioWu_dave		11/25/13 12:24:05.000	
🕨 🌔	brioWuPar		10/23/13 14:08:20.000	
🕨 🌔	collisionalMultiFluid		10/21/13 12:02:09.000	
🕨 🌔	collisionalMultiFluid1		10/22/13 15:45:01.000	
▶ 🕼	densePlasmaFocus		10/22/13 15:45:20.000	
Filter b	y: Runspace Files			\$
				Cancel Open

Fig. 2.39: Open Runspace window



Fig. 2.40: Select Edit menu



Fig. 2.41: Select Settings from the Tools menu

General

00	U Application Settings
General Host Settings Editor	When opening a runspace with existing data Ask before opening visualization +
Visualization Options License	When starting run on a runspace with existing data Ask before deleting existing data ‡
	When opening a runspace when another runspace is already opened
	Ask before saving files and command line options of existing runspace 🗘
Apply	Cancel OK

General Application Settings apply to default behavior for the USimComposer applications such as file and directory actions.

Fig. 2.42: General Application Settings

The default setting that USimComposer will use when opening a runspace with existing data is *Ask before opening visualization*. If you know that you will always want to visualize data whenever it is available, you may use the pulldown menu to set the default to *Always open visualization*. If you prefer to indicate whenever you want to visualize existing data by using the **Visualize** icon yourself instead of having USimComposer open the visualization of existing data for you, you may use the pulldown menu to set the default to set the default to or *Never open visualization*.

The default setting that USimComposer will use when starting a run on a runspace that already contains data is *Ask* before deleting existing data. If you know that you will always want to create fresh data for each run, use the pulldown menu to set the default to *Always delete existing data*. If you know that you will always want to run on the data already available, use the pulldown menu to set the default to *Never delete existing data*.

The default setting that USimComposer will use when opeing a runspace while another runspace is already opened is *Ask before saving files and command line options of existing runspace*. If you know that you will alaways want to save the runspace this can be switched to *Always save files and command line options of existing runspace*. If you know that you will never want to save the runspace this can be switched to *Never save files and command line options of existing runspace*. If *you know that you will never want to save the runspace this can be switched to Never save files and command line options of existing runspace*.



Fig. 2.43: Application Setting When Opening Runspace with Existing Data



Fig. 2.44: Application Setting When Starting Run on a Runspace with Existing Data

$\Theta \cap \Theta$	U Application Settings
General Host Settings Editor Visualization Options License	When opening a runspace with existing dataAsk before opening visualization \$When starting run on a runspace with existing dataAsk before deleting existing data \$
	When opening a runspace when another runspace is already opened
	 ✓ Ask before saving files and command line options of existing runspace Always save files and command line options of existing runspace Never save files and command line options of existing runspace
Apply	Cancel

Fig. 2.45: Application Setting When Opening a Runspace When Another Runspace is Already Open

Host Settings

Paths

The default path that USimComposer will use as the top level directory to which to add runspace directories is displayed in the Host Settings window underneath the *Paths* tab in the *Workspace Directory* field. You can type in another path if you so wish.

The USimComposer Installation Directory is used to let USimComposer know the correct paths to the Ulixes executables as well as other paths to allow USim to work.

MPI

By default, USim runs in serial mode. If you have a multi-core system capable of parallel processing, you can set the default to parallel instead of serial by clicking on the *Preferred Run Method* drop down menu and selecting parallel.

USimComposer detects the number of available cores for the system on which it is running and lists this value in the **Cores On Machine** field.

USimComposer reads the USim license file and sets the default number of **Cores In License** to match the number of cores specified in the license file. If you would like to run simulations using fewer processes than the number of cores for which your software is licensed or perhaps try some load balancing using more processes than you have cores, you may change the number of cores by entering a new value in the **Preferred Number of Cores** field. When the value in the **Preferred Number of Cores** field is set to something other than the last saved value, USimComposer places an asterisk in front of the field label so that you are aware that you have changed the value and may wish to save the new value.

00	U Арр	lication Settings
General Host Settings	Profiles	General Paths MPI
Editor Visualization Options	localhost	Preferred run method: Serial +
License		Cores in license: 2
		Cores on machine: 4
		Preferred number of cores: 2
	Add Remove	
Apply		Cancel OK

Fig. 2.46: Application Setting Engine Menu

Editor

The editor tab contains default settings for font and font size. These are editable to the users desired settings. Any file with the extensions listed in the *Extensions* box will use the settings under *Files with Fixed-width Font* and all other files under the *All Other Files* sections.

Visualization Options

The visualization options tab allows the user control over default settings of the *Visualize* tab in USimComposer. By checking *Manual font sizing* the size of the fonts can be controlled. If *Enable VisIt context menu* is selected it will be possible to right click on the visualization and open VisIt itself allowing the user access to every function and feature of VisIt. It also enables the embedded point and line tools in VisIt as well as some of the generic view controls.

License Settings

It is possible to review your USim license, as well as install a new license if an upgrade or additional packages are purchased.

To install a new license click on the Add button and navigate to where your new license is located, and hit ok.

	U Applic	tation Settings	
General Host Settings Editor Visualization Options License	Files with Fixed-width Font Extensions py pre in Font Courier New Size 12 All Other Files Font Verdana Size 12		+
	Tabstop Width 2 \$ ✓ Open files in "Parameter" edito ✓ Use syntax highlighting ✓ Show line numbers ✓ Highlight current line ✓ Show post-processed file ✓ Word wrap	r by default	
Apply		Cancel	OK

Fig. 2.47: Editor Menu

000	U Application Settings
General Host Settings	Manual font sizing
Editor Visualization Options License	
	Automatic Font Size: Medium +
	Enable Vislt context menu
	Iry harder to load cycles and times (Requires Restart)
Apply	Cancel OK

Fig. 2.48: Visualization Menu



Fig. 2.49: License Settings Dialog

CHAPTER

THREE

USIMBASE EXAMPLES

The USimBase examples demonstrate the basic solvers available in USim. The USimBase examples can be executed with a USimBase license.

3.1 Flow over a Forward-Facing Step (forwardFacingStep.pre)

Keywords:

hydrodynamics, unstructured mesh, supersonic flow, shock wave generation, Forward-Facing St

3.1.1 Problem description

This problem demonstrates supersonic flow over a forward-facing step, involving Mach 3 flow at an inlet to a rectangular domain. A step is placed near the inlet region that generates shock waves. An unstructured mesh, with a reflecting wall boundary at the step, is used in this example.

This simulation can be performed with a USimBase license.

3.1.2 Creating the run space

The Flow over a Forward-Facing Step example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Flow over a Forward-Facing Step and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as shown below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.1.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for the Flow over a Forward-Facing Step.

The following parameters control the physics:

- *MHD* = *False*, *True* selects whether to evolve the problem in the inviscid hydrodynamic limit (*MHD* = False) or the ideal magnetohydrodynamic limit (*MHD* = True).
- *BETA* controls the ratio of the gas pressure to the magnetic pressure for problems solved in the magnetohydrodynamic limit (i.e. when *MHD* = True).
- GAS_GAMMA sets the adiabatic index (ratio of specific heats) of the fluid.
- GRIDFILE Mesh file to use
- *GRIDFORMAT* Format of the mesh file (either ExodusII or Gmsh)

The following parameters the length of the simulation and data output:

- *TEND* sets the end time for the simulation.
- *NUMDUMPS* sets the number of data dumps during the simulation
- *WRITE_RESTART = False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to *False* then the *Restart at Dump Number* functionality in the *Standard* tab under *Runtime Options* in the *Run* window will not be available.

The following parameters control the USim solvers used to evolve the simulation:

- *TIME_ORDER = first, second, third, fourth* sets the order of accuracy for the time-integration.
- DIFFUSIVE = False, True sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG = False,True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.1.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.1.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Geometries* in the *Visualization Controls* pane and click the checkbox for *fluids/forwardFacingStep* to visualize simulation geometry.
- Expand Scalar Data and click the check box for *fluids/density* to visualize fluid densities.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The fluid density distribution at the end of the simulation is shown in Fig. 3.1.



Fig. 3.1: Visualization of the Flow over a Forward-Facing Step example using a color contour plot

3.1.6 Further experiments

Several Gmsh format mesh files are included with this example. The default file choice is "forwardFacingStep.msh", which is a low-resolution mesh partitioned for serial execution. Higher-resolution meshes (*forwardFacingStep2.msh*, *forwardFacingStep8.msh*) are included for 2, 4, and 8 core runs, respectively. To run the example using the 2-core mesh, proceed as follows:

- Return to the Setup window by pressing the Setup icon in the workflow panel.
- Enter the mesh file name "forwardFacingStep2.msh" in the GRIDFILE text box.
- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- In the Run window, press the MPI tab in the Runtime Options pane.
- Check the box marked Run with MPI and set Number of Cores equal to 2.
- To run the simulation, click on the *Run* button in the upper right corner of the *Logs and Output Files* pane. You will again see the engine output in the *Logs and Output Files* pane'.

After the simulation has executed, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Geometries* in the *Visualization Controls* pane and click the checkbox for *fluids/forwardFacingStep* to visualize simulation geometry.
- Expand Scalar Data and click the check box for fluids/density to visualize fluid densities.

• Drag the slider at the bottom of the Visualization Results pane to move through the simulation in time.

3.2 Kelvin-Helmholtz Instability (khlnstability.pre)

Keywords:

hydrodynamics, Kelvin-Helmholtz Instability

3.2.1 Problem description

This problem demonstrates the Kelvin-Helmholtz instability for the case of a velocity difference across the interface between two different fluids that differ in density by a factor 2. A finite-width shear layer is used to ensure results converge at finite resolution. For the two-dimensional version of the problem setup considered here, we use a domain

 $(-PAR_{LENGTH}/2, -PERP_{LENGTH}/2) \times (PAR_{LENGTH}/2, PERP_{LENGTH}/2)$

with periodic boundary conditions in the *PAR* direction and reflecting wall boundary conditions in the *PERP* direction. For the three-dimensional version of the problem setup considered here, we use a domain

 $(-PAR_{LENGTH}/2, -PERP_{LENGTH}/2, -PAR_{LENGTH}/2) \times (PAR_{LENGTH}/2, PERP_{LENGTH}/2, PAR_{LENGTH}/2) \times (PAR_{LENGTH}/2, -PAR_{LENGTH}/2, -PAR_{LENGTH}/2) \times (PAR_{LENGTH}/2, -PAR_{LENGTH}/2) \times (PAR_{LENGTH}/2) \times (PAR$

with periodic boundary conditions in the *PAR* directions and reflecting wall boundary conditions in the *PERP* direction. A single mode perturbation is used to seed the instability.

This simulation can be performed with a USimBase license.

3.2.2 Creating the run space

The Kelvin-Helmholtz Instability example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Kelvin-Helmholtz Instability and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as shown below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.2.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for the Kelvin-Helmholtz instability.

The following parameters control the physics of the Kelvin-Helmholtz instability:

- *MHD* = *False*, *True* selects whether to evolve the problem in the inviscid hydrodynamic limit (*MHD* = False) or the ideal magnetohydrodynamic limit (*MHD* = True).
- *MACH_NUM* sets the ratio of the flow velocity to the sound speed (the Mach number). Note that the Kelvin-Helmholtz instability is stabilized for Mach Numbers greater than unity.

- *BETA* controls the ratio of the gas pressure to the magnetic pressure for problems solved in the magnetohydrodynamic limit (i.e. when *MHD* = True). Note that, for strong enough magnetic fields (small enough *BETA*), the Kelvin-Helmholtz instability is stabilized.
- GAS_GAMMA sets the adiabatic index (ratio of specific heats) of the fluid.

The following parameters control the shear layer that drives Kelvin-Helmholtz instability and the perturbation used to seed the Kelvin-Helmholtz instability:

- *SHEAR_LAYER_WIDTH* sets the width of the shear layer. This should be resolved by 2-3 cells on the mesh in order for the instability to grow.
- *PERTURB_AMP* sets the strength of the perturbation, seeding the instability relative to the flow velocity.
- *PERTURB_WIDTH* sets the spatial width of the perturbation that seeds the instability.

The following parameters control the dimensionality, domain size and resolution of the simulation:

- NDIM = 2,3 selects whether to run the problem in two- or three-dimensions.
- PAR_LENGTH sets the size of the domain in the direction parallel to the shear layer.
- *PERP_LENGTH* sets the size of the domain in the direction perpendicular to the shear layer.
- PAR_ZONES sets the number of zones in the direction parallel to the shear layer.
- *PERP_ZONES* sets the number of zones in the direction perpendicular to the shear layer.

The following parameters the length of the simulation and data output:

- *TEND* sets the end time for the simulation.
- *NUMDUMPS* sets the number of data dumps during the simulation
- *WRITE_RESTART = False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to *False* then the *Restart at Dump Number* functionality in the *Standard* tab under *Runtime Options* in the *Run* window will not be available.

The following parameters control the USim solvers used to evolve the Kelvin-Helmholtz instability:

- TIME_ORDER = first, second, third, fourth sets the order of accuracy for the time-integration.
- *DIFFUSIVE* = *False*,*True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG = False,True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.2.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.2.5 Visualizing the results

After performing the above actions, continue as follows:

• Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.

- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/density to visualize fluid densities.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The density of the Kelvin-Helmholtz instability at the end of the simulation is shown in Fig. 3.2.



Fig. 3.2: Visualization of the density in the Kelvin-Helmholtz Instability example

3.2.6 Further experiments

- Set *MHD* to *True* to solve the magnetized Kelvin-Helmholtz instability, which demonstrates USim capabilities to amplify magnetic fields.
- Set *TIME_ORDER* to *third* or *fourth* to see the effect of increased temporal accuracy on the Kelvin-Helmholtz instability.
- Set *NDIM* to *3* to solve the Kelvin-Helmholtz instability in 3D. The increased computational requirements of such a simulation means that you should enable *Run with MPI* in the *MPI* tab under *Runtime Options* in the *Run Window*.

3.3 Magnetized Ramp Flow (rampFlow.pre)

Keywords:

body fitted grid, MHD, ramp flow, supersonic

3.3.1 Problem description

This simulation shows magnetized flow over a ramp using ideal magnetohydrodynamics. The shock wave leads to compression of both the fluid and the magnetic field.

This simulation can be performed with a USimBase license.

3.3.2 Creating the run space

The Magnetized Ramp Flow example is accessed from within USimComposer by the following actions:

- Select the *New from Template* menu item in the *File* menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Magnetized Ramp Flow and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as described below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.3.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for the magnetized ramp flow problem.

The following parameters control the physics of the magnetized ramp flow problem:

- *THETA* controls the angle of attack of the ramp.
- PRESSURE controls the pressure of the inflowing fluid.
- DENSITY controls the density of the inflowing fluid.
- MACH_NUM sets the ratio of the flow velocity to the sound speed (the Mach number) for the inflowing gas.
- BETA controls the ratio of the gas pressure to the magnetic pressure in the inflowing gas.
- GAS_GAMMA sets the adiabatic index (ratio of specific heats) of the fluid.

The following parameters control the dimensionality, domain size and resolution of the simulation:

- NDIM = 2,3 selects whether to run the problem in two- or three-dimensions.
- *SCALE* sets the resolution of the grid. Large values correspond to higher resolution.

The following parameters control the duration of the simulation and data output:

- TEND sets the end time for the simulation
- *NUMDUMPS* sets the number of data dumps during the simulation

• *WRITE_RESTART = False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to *False* then the *Restart at Dump Number* functionality in the *Standard* tab under *Runtime Options* in the *Run* window will not be available.

The following parameters control the USim solvers used to run the simulation:

- TIME_ORDER = first, second, third, fourth sets the order of accuracy for the time-integration.
- *DIFFUSIVE* = *False*,*True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG = False,True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.3.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.3.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/density to visualize fluid density.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The density at the end of the simulation is shown in Fig. 3.3.

3.3.6 Further experiments

- You can increase the steepness of the shock by reducing the Mach number (MACH_NUM).
- You can also change the angle of the shock by changing the ramp angle (*THETA*).
- Set *NDIM* to *3* to solve the magnetized ramp flow problem in 3D. The increased computational requirements of such a simulation means that you should enable *Run with MPI* in the *MPI* tab under *Runtime Options* in the *Run Window*.

3.4 Rayleigh-Taylor Instability (rtInstability.pre)

Keywords:

hydrodynamics, gravitational force, Rayleigh Taylor Instability



Fig. 3.3: Visualization of the fluid mass density in the Magnetized Ramp Flow example

3.4.1 Problem description

This problem demonstrates the Rayleigh-Taylor instability for the case of a heavy fluid on top of a lighter fluid, subject to a constant gravitational acceleration. The pressure is determined by the conditions of hydrostatic equilibrium. For the two-dimensional version of the problem setup considered here, we use a domain

 $(-TRANS_{LENGTH}/2, -PAR_{LENGTH}/2) \times (TRANS_{LENGTH}/2, PAR_{LENGTH}/2)$

with periodic boundary conditions in the *TRANS* direction and reflecting wall boundary conditions in the *PAR* direction. For the three-dimensional version of the problem setup considered here, we use a domain

 $(-TRANS_{LENGTH}/2, -PAR_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, PAR_{LENGTH}/2, TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -PAR_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2, -TRANS_{LENGTH}/2) \times (TRANS_{LENGTH}/2) \times (TRA$

with periodic boundary conditions in the *TRANS* directions and reflecting wall boundary conditions in the *PAR* direction. A single mode perturbation is used to seed the instability.

This simulation can be performed with a USimBase license.

3.4.2 Creating the run space

The Rayleigh-Taylor Instability example is accessed from within USimComposer by the following actions:

- Select the *New from Template* menu item in the *File* menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Rayleigh-Taylor Instability and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as shown below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.4.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for the Rayleigh-Taylor instability.

The following parameters control the physics of the Rayleigh-Taylor instability:

- GRAVITY_ACCEL sets the acceleration due to gravity.
- *RHO_LIGHT* sets the density of the lighter fluid initially at the bottom of the domain.
- *RHO_HEAVY* sets the density of the heavier fluid initially at the top of the domain.
- GAS_GAMMA sets the adiabatic index (ratio of specific heats) of the fluid.
- *PERTURB_AMP* sets the strength of the perturbation seeding the instability.
- *MHD* = *False*, *True* selects whether to evolve the problem in the inviscid hydrodynamic limit (*MHD* = False) or the ideal magnetohydrodynamic limit (*MHD* = True).
- *BETA* controls the ratio of the gas pressure to the magnetic pressure for problems solved in the magnetohydrodynamic limit (i.e. when *MHD* = True). Note that, for strong enough magnetic fields (small enough *BETA*), the instability is stabilized.

The following parameters control the dimensionality, domain size and resolution of the simulation:

• NDIM = 2,3 selects whether to run the problem in two-dimensions or three-dimensions.

- PAR_LENGTH sets the size of the domain in the direction parallel to the gravitational acceleration vector.
- TRANS_LENGTH sets the size of the domain in the direction transverse to the gravitational acceleration vector.
- PAR_ZONES sets the number of zones in the direction parallel to the gravitational acceleration vector.
- TRANS_ZONES sets the number of zones in the direction transverse to the gravitational acceleration vector.

The following parameters the length of the simulation and data output:

- TEND sets the end time for the simulation
- NUMDUMPS sets the number of data dumps during the simulation
- *WRITE_RESTART = False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to *False* then the *Restart at Dump Number* functionality in the *Standard* tab under *Runtime Options* in the *Run* window will not be available.

The following parameters control the USim solvers used to run the simulation:

- *TIME_ORDER = first, second, third, fourth* sets the order of accuracy for the time-integration.
- *DIFFUSIVE* = *False*,*True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG = False,True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.4.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.4.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize button in the left column of buttons.
- Press the "Open" button to begin visualizing.
- To visualize the fluid density, expand the Scalar Data tab and click the check box for fluids/density.
- Drag the slider at the bottom of the visualization window to move through the simulation in time. The fluid density distribution at the end of the simulation is shown in Fig. 3.4.

3.4.6 Further experiments

- Set *MHD* to *True* to solve the magnetized Rayleigh-Taylor instability.
- Set *TIME_ORDER* to *third* or *fourth* to see the effect of increased temporal accuracy on the Rayleigh-Taylor instability.
- Set *NDIM* to 3 to solve the Rayleigh-Taylor instability in 3D. The increased computational requirements of such a simulation means that you should enable *Run with MPI* in the *MPI* tab under *Runtime Options* in the *Run Window*.



Fig. 3.4: Visualization of density in the Rayleigh-Taylor instability example as a color contour plot.

3.5 Shock Tube (shockTube.pre)

Keywords:

hydrodynamics, magnetohydrodynamics, Riemann problem, shock tube

3.5.1 Problem description

This example computes shock tube problems for both hydrodynamic and magnetized flows. In essence, a shock tube is a 1D Riemann problem driven by discontinuous left and right states. Here, we provide a range of specific shock tubes for an ideal gas, including examples due to Einfeldt, Sod, Liska & Wendroff, Brio & Wu and Ryu & Jones. Further details, including reference solutions can be found in Stone et al. The Astrophysical Journal Supplement Series, Volume 178, Issue 1, article id. 137-177, pp. (2008).

This simulation can be performed with a USimBase license.

3.5.2 Creating the run space

The Shock Tube example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select *Shock Tube* and press the *Choose* button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as described below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.5.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for solving a shock tube problem.

The following parameters control the initial conditions of the shock tube:

- SHOCK_TUBE = EINFELDT1125, EINFELDT1203, SOD, SODLEVEQUE, SODTORO, LISKAWENDROFF, SLOW, BRIOWU, RYUJONES1a, RYUJONES1b, RYUJONES2a, RYUJONES2b, RYUJONES3a, RYUJONES3b, RYUJONES4a, RYUJONES4b, RYUJONES4c, RYUJONES4d selects the initial condition to run.
- REFERENCE_PRESSURE Pressure to scale the solution by in order to set the global sound speed.
- *REFERENCE_DENSITY* Density to scale the solution by in order to set the global sound speed.
- GAS_GAMMA Adiabatic index, or ratio of specific heats
- *MU0* Vacuum permeability

The following parameters control the dimensionality, domain size and resolution of the simulation:

- NDIM = 1,2,3 selects whether to run the problem in one-, two- or three-dimensions.
- *PAR_LENGTH* sets the size of the domain in the direction parallel to the shock.
- *PERP_LENGTH* sets the size of the domain in the direction perpendicular to the shock.

- PAR_ZONES sets the number of zones in the direction parallel to the shock.
- *PERP_ZONES* sets the number of zones in the direction perpendicular to the shock.

The following parameters the length of the simulation and data output:

- *TEND* sets the end time for the simulation.
- NUMDUMPS sets the number of data dumps during the simulation
- WRITE_RESTART = False, True tells USim to output data necessary to restart the simulation. If this parameter is set to False then the Restart at Dump Number functionality in the Standard tab under Runtime Options in the Run window will not be available.

The following parameters control the USim solvers used to evolve the Kelvin-Helmholtz instability:

- *TIME_ORDER = first, second, third, fourth* sets the order of accuracy for the time-integration.
- *DIFFUSIVE = False,True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG = False,True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.5.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the *Run* window as instructed by pressing the *Run* icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.5.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Navigate to the "1-D Fields" Data View
- The visualization opens with four panels consisting of 1D line plots. The quantities are 'fluids/density' (mass density), 'fluids/pressure' (thermal pressure), 'fluids/velocity_0', 'fluids/velocity_1', 'fluids/velocity_2' (three components of the fluid velocity)
- Drag the slider at the bottom of the *Visualization Results* pane to Dump 10 to see results at the end of the simulation, as shown in Fig. 3.5.

3.5.6 Further experiments

- Change the adiabatic index of the gas (GAS_GAMMA) to see the effect of the gas having an different equation of state.
- Change the number of times a sound wave crosses the box (*WAVE_CROSSINGS*) to see the discontinuities propagate through the volume.
- Change the initial condition (*SHOCK_TUBE*) to the classic magnetized Brio & Wu shock tube (*SHOCK_TUBE* = *BRIOWU*).



Fig. 3.5: Visualization of gas pressure, fluid density and first component of the velocity for the default Shock Tube example.

Drag the slider at the bottom of the *Visualization Results* pane to Dump 10 to see results at the end of the simulation, as shown in Fig. 3.6.



Fig. 3.6: Visualization of gas pressure, fluid density and velocity for the default Brio & Wu shock tube.

3.6 Unstable Plasma zPinch (zPinch.pre)

Keywords: MHD, ideal plasma instabilities

zPinch

3.6.1 Problem description

The Z-Pinch is an ideal MHD simulation of a cylindrical plasma with a purely axial current and a periodic boundary condition in the axial direction. This problem uses a top-hat current density profile such that

$$\mathbf{J} = \begin{cases} J_0 \hat{z} & r \le r_p \\ 0 & r > r_p \end{cases}$$

where r_p is the current column radius. Thus, the magnetic field is

$$\mathbf{B} = \begin{cases} -\frac{r}{2}\mu_0 J_0 \hat{\theta} & r \leq r_p \\ -\frac{r_p^2}{2r}\mu_0 J_0 \hat{\theta} & r > r_p \end{cases}$$

The MHD force balance condition $(\mathbf{J} \times \mathbf{B} = \nabla p)$ becomes

$$\frac{dp}{dr} + \frac{B_{\theta}}{\mu_0 r} \frac{d}{dr} \left(r B_{\theta} \right)$$

and, thus, the pressure profile is

$$p = \begin{cases} \frac{\mu_0 J_0^2}{4} \left[(1+\alpha) r_p^2 - r^2 \right] & r \le r_p \\ \frac{\mu_0 J_0^2}{4} \alpha r_p^2 & r > r_p \end{cases}$$

where α sets the base pressure outside the plasma column.

In general, the plasma column may be unstable to perturbations with a wavenumber (k) such that

$$\mathbf{k} = \frac{m}{r}\hat{\theta} + \frac{2\pi n}{Z}\hat{z}$$

where m is the azimuthal wavenumber, n is the axial wavenumber, and Z is the axial length of the computational domain. This example assumes axisymmetry in the azimuthal direction of the cylindrical column, and thus instabilities with m = 0 are modeled. The simulation is initialized with a n = 1 perturbation in the magnetic field which leads to instability with the default parameters.

This simulation can be performed with a USimBase license.

3.6.2 Creating the run space

The Unstable Plasma Z-Pinch example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Unstable Plasma Z-Pinch and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as described below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

3.6.3 Input file features

The key variables of the input file are exposed in the *Setup* window. These variables allow one to set the following fields:

The following parameters control the physics of the Z-Pinch:

- AXIAL_LENGTH The axial length of the cylinder.
- CURRENT The axial current in the plasma column $(I = J_0 \pi r_p^2)$.
- NUM_MODES Sets the wavenumber
- *BASE_PRESSURE_RATIO* The ratio of the pressure and density at the wall to the pressure and density in the plasma core (α).
- *PERTURBATION_AMPLITUDE* The relative amplitude of the perturbed field to the field generated by the axial current.
- GAS_GAMMA The ratio of specific heats

The following parameters control the dimensionality, domain size and resolution of the simulation:

- *RADIAL_RESOLUTION* The number of radial grid points.
- AXIAL_RESOLUTION The number of axial grid points.

The following parameters the length of the simulation and data output:

- *TEND* sets the end time for the simulation.
- NUMDUMPS sets the number of data dumps during the simulation
- *WRITE_RESTART* = *False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to *False* then the *Restart at Dump Number* functionality in the *Standard* tab under *Runtime Options* in the *Run* window will not be available.

The following parameters control the USim solvers used to evolve the Z-Pinch:

- *TIME_ORDER = first, second, third, fourth* sets the order of accuracy for the time-integration.
- *DIFFUSIVE* = *False*,*True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG* = *False*,*True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

3.6.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

3.6.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing. Select a Data View of Field Analysis.
- Select *fluids/density* from the *Field* dropdown.
- Click the check box for Log Scale Color Table to view the density using a logarithmic scale.
- Drag the slider at the bottom of the *Visualization Results* pane to see results for the different simulation data dumps, as shown in Fig. 3.7.
- Add a corresponding line plot by adjusting settings in the *Lineout Settings* pane and pressing the *Perform Lineout* button to draw.

The plot in Fig. 3.7 was made with the calewhite color scale at time 3×10^{-6} seconds. Here the instability is in the nonlinear phase, and the plasma density has ruptured out of the initial plasma column.


Fig. 3.7: Visualization of the mass density in the Unstable Plasma Z-Pinch example

3.6.6 Further experiments

• Run the computation into the deep nonlinear stage at current resolution, then run it again with decreased or enhanced resolution. Note there is no dissipation in the ideal MHD system so differing results are expected when dynamics are on the grid-scale length.

CHAPTER

USIMHEDP EXAMPLES

The USimHEDP examples illustrate how to solve complex problems in high energy density plasmas. The USimHEDP examples can be executed with a USimHEDP license.

4.1 Anisotropic Diffusion (anisotropicDiffusion.pre)

Keywords:

Anisotropic Diffusion

4.1.1 Problem description

This example simulates anisotropic diffusion where the conductivity is high parallel to circular rings and low perpendicular to this rings.

This simulation can be performed with a USimHEDP license.

4.1.2 Creating the run space

The Anisotropic Diffusion example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Anisotropic Diffusion and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.1.3 Input file features

The following parameters can be varied to study different plasmas:

- KPARALLEL Conductivity in parallel direction
- *KPERPENDICULAR* Conductivity in perpendicular direction

- CFL Explicit CFL
- CFLSTEP Super Time Stepping CFL
- *TIME_ORDER = first, second, third, fourth* sets the order of accuracy for the time-integration
- *GRIDFILE* Name of the grid file (*anisotropicDiffusion.msh* for serial, *anisotropicDiffusion2.msh* for parallel run on 2 cores)
- GRIDFORMAT Format of mesh file (either ExodusII or Gmsh)
- TEND Simulation end time (seconds)
- NUMDUMPS Number of data dumps during the simulation
- *WRITE_RESTART = False,True* tells USim to output data necessary to restart the simulation. If this parameter is set to False then the Restart at Dump Number functionality in the Standard tab under Runtime Options in the Run window will not be available.
- *DIFFUSIVE* = *False*,*True* sets whether to use diffusive (but robust!) spatial integration schemes.
- *DEBUG* = *False*,*True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

4.1.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.1.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/pressure to visualize the fluid pressure.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The pressure distribution at the end of the simulation is shown in Fig. 4.1.

4.1.6 Further experiments

• Try varying KPARALLEL. Increasing the value should result in faster diffusion of the transport parameter.

4.2 Anisotropic Poisson (anisotropicPoisson.pre)

Keywords:

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iterative, multigrid, Poisson, electrostatics, magnetostatics
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Fig. 4.1: Visualization of fluid pressure for the Anisotropic Diffusion example

4.2.1 Problem description

This example demonstrates the anisotropic Poisson solve that can be used for the electric potential, heat transfer, magnetic field diffusion, and wherever a Poisson's equation has to be solved. A source varying in space and time is considered. The source has a sine wave variation at a frequency of 1 MHz. The coefficients are assumed to be different in x,y, and z directions. Source is given by s = (6x+12y+18z)*sin(wt). Simulation is performed for a duration of one cycle. For CX=1, CY=2, and CZ=3, the result would be $x^3+y^3+z^3$.

This simulation can be performed with a USimHEDP license.

4.2.2 Creating the run space

The Anisotropic Poisson example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Anisotropic Poisson and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.2.3 Input file features

Primary variables are:

- FREQUENCY source variation frequency
- CX, CY, CZ coefficients in the x,y,z directions
- NX, NY, NZ Number of cells in the x,y,z directions
- *NUMDUMPS* Number of data dumps during the simulation

4.2.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.2.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the *Open* button to begin visualizing. The left pane has all of the output variable from the simulation. Expand the 'Scalar Data' field to see 'fluids/coeff_0..._9' (tensor of the diffusion coefficients), phi (scalar potential), and rho (source on the right hand side of the Poisson's equation).
- Select the variable 'phi' and drag the slider at the bottom of the *Visualization Results* pane to the right to see potential at the positive peak of the source simulation. Check the 'Display Contour' option and hold+move the cursor along the contours to set an orientation as shown in Fig. 4.2.

4.2.6 Further experiments

• Change the resolution of the grid by setting NX, NY, NZ to 64 or 128 to see more refined results.

4.3 Multi-Fluids with Collisions (collisionalMultiFluid.pre)

Keywords:

Multi-Fluid Collisions

4.3.1 Problem description

This problem shows collisions between three (separate) fluid species in a simple shock problem and allows one to compare it with the single-fluid solution. In the highly collisional regime the multi-fluid problem converges to the single fluid case.

This simulation can be performed with a USimHEDP license.



Fig. 4.2: Visualization of the time varying scalar potential

4.3.2 Creating the run space

The Multi-Fluids with Collisions example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Multi-Fluids with Collisions and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.3.3 Input file features

The following parameters can be varied to look at the effects of collisionality on the shock solution:

- NUMDUMPS Number of data dumps during the simulation
- XUPPER Domain size
- PRESSURE Reference pressure of the gas
- DENSITY Reference density of the gas
- GAMMA Gas constant
- *PRL* the total pressure on the left half of the domain.
- *RHOL* the total density on the left half of the domain.
- *PRR* the total pressure on the right half of the domain.
- *RHOR* the total density on the right half of the domain.
- *FRAC1L* the fraction of gas 1 on the left half initially.
- *FRAC2L* the fraction of gas 2 on the left half initially.
- *FRAC3L* the fraction of gas 3 on the left half initially.
- FRAC1R the fraction of gas 1 on the right half initially.
- FRAC2R the fraction of gas 2 on the right half initially.
- FRAC3R the fraction of gas 3 on the right half initially.
- MI Reference mass of ion
- DI Reference diameter of ion
- *MI1* Mass of ion1
- MI2 Mass of ion2
- MI3 Mass of ion3
- DI1 Diameter of ion1
- *DI2* Diameter of ion2
- DI3 Diameter of ion3

4.3.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.3.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing. The visualization opens with four panels consisting of 1D line plots.
- Drag the slider at the bottom of the *Visualization Results* pane to see results at the end of the simulation, as shown in Fig. **??**.

The following values can be visualized

- *N1,N2,N3* the number densities for species 1, 2 and 3
- *T1,T2,T3* the temperatures for species 1, 2 and 3
- *V1_0,V1_1,V1_2* the velocity components for species 1
- *V2_0,V2_1,V2_2* the velocity components for species 2
- V3_0, V3_1, V3_2 the velocity components for species 3
- collisionMatrix_0 through collisionMatrix_8 the collisional cross frequencies between species
- q1_0,q1_1,q1_2,q1_3,q1_4 the mass density, momentum density and energy of the first species
- q2_0,q2_1,q2_2,q2_3,q2_4 the mass density, momentum density and energy of the second species
- q3_0,q3_1,q3_2,q3_3,q3_4 the mass density, momentum density and energy of the third species
- *qTotal_0,qTotal_1,qTotal_2,qTotal_3,qTotal_4* the mass density, momentum density and energy of the sum of the 3 species

4.3.6 Further experiments

• Increase *RHOL* and *RHOR* by a factor of 10 and the fluids will become much more collisional, producing the standard sod shock result.

4.4 Dense Plasma Focus (densePlasmaFocus.pre)

Keywords:

Z-pinch, dense plasma focus, MHD, axisymmetric, MPD, two temperature, general equation of a



Fig. 4.3: Visualization of the densities of each species and the temperature of the first species for the Multi-Fluids with Collisions example

4.4.1 Problem description

This problem solves a simple dense plasma focus (DPF) using a two-temperature MHD model with a user-specified equation of state on an unstructured grid in axisymmetric geometry. The dense plasma focus is a fusion concept envisioned as both a power source, neutron source, and even high-powered propulsion. The DPF is also similar to other plasma accelerators such as the magneto plasma dynamic (MPD) thruster, in which the plasma is accelerated by the self field created by the current running through the plasma.

4.4.2 Creating the run space

The Dense Plasma Focus example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Dense Plasma Focus and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.4.3 Input file features

The input file allows the user to specify the number density of the plasma (N0), the temperature of the plasma (T), a constant resistivity (*ETA*), the atomic weight of the plasma species (*ATOMIC_WEIGHT*), and the current flowing through the plasma (*CURRENT*). In addition, many numerical parameters can be set through the input file.

The key variables of the input file are exposed in the "Setup" window. These variables allow one to set the following fields

- *GRIDFILE* Name of the mesh file
- CFL CFL condition for the simulation
- TEND Simulation end time (seconds).
- *NUMDUMPS* Number of data dumps during the simulation
- ATOMIC_WEIGHT Atomic weight of ion
- *ION_TEMP* The temperature of the ions (Kelvin)
- TEMPERATURE_RATIO Temperature ratio of electrons and ions at the nozzel inlet
- *CURRENT* The current flowing through the plasma (Amps)
- *N0* The peak ion number density (number/m³)
- *OHMIC_RESISTIVITY* The resistivity of the plasma (constant Ohm Meters)
- *NUMERICAL_FLUX* specifies the Riemann solver used to calculate an upwind approximation to the flux tensor. For hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, hlleFlux. For magnetohydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, fWaveFlux. For more general systems, options include localLaxFlux, hlleFlux, fWaveFlux.
- *TIME_ORDER=first, second, third, fourth* sets the order of accuracy for the time-integration.
- *LIMITER=muscl,minmod,none* specifices the spatial limiting method used in reconstructing primary variables to use to ensure that method remains total value diminishing (TVD).
- VARIABLE_FORM Limit in primitive or conservative variables

4.4.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.4.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for *fluids/q_0* to visualize the mass density of the plasma.

• Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The results near the end of the simulation are shown in Fig. 4.4.



Fig. 4.4: Visualization of mass density in the Dense Plasma Focus example

4.4.6 Further experiments

Two ExodusII format mesh files are included with this example. The default file choice is "dpf.g", which is a mesh partitioned for serial execution. Additional meshes (*dpf.g.2.**, *dpf.g.4.**, *dpf.g.8.**) are included for 2, 4, and 8 core runs, respectively. Unlike GMSH meshes, it is not necessary to specify the number of cores that the mesh is partioned onto; USim looks for the appropriate files automatically. To run the example using the 2-core mesh, proceed as follows:

- Return to the Run window by pressing the Run icon in the workflow panel.
- In the Run window, press the MPI tab in the Runtime Options pane.
- Check the box marked *Run with MPI* and set *Number of Cores* equal to 2.
- To run the simulation, click on the *Run* button in the upper right corner of the *Logs and Output Files* pane. You will again see the engine output in the *Logs and Output Files* pane'.

After the simulation has executed, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Geometries* in the *Visualization Controls* pane and click the checkbox for *fluids/domain* to visualize simulation geometry.
- Expand *Scalar Data* and click the check box for *fluids/q_0* to visualize fluid densities.

• Drag the slider at the bottom of the Visualization Results pane to move through the simulation in time.

We can run further experiments on the dense plasma focus. For example, we can explore the effect of increasing the current (CURRENT) or decreasing the number density (N0). In the latter case, the plasma should move faster.

4.5 Gas Injection (gasInjection.pre)

Keywords:

hydrodynamics, vacuum, boundary

4.5.1 Problem description

This problem not only demonstrates the time-dependent boundary condition capabilities in USim, but also the ability to handle extremely strong shocks in 3 dimensions. In this case, the injected fluid is 6 orders of magnitude more dense than the background gas.

4.5.2 Creating the run space

The Gas Injection example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimBase: Basic Physics Capabilities.
- Select Gas Injection and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.5.3 Input file features

The input file allows the user to set the jet pressure (*PRESSURE*), the jet mass density (*RHO*), the jet flow velocity (*U*), the cfl number (*CFL*), the end time (*TEND*), and the number of data dumps (*NUMDUMPS*).

Primary variables are:

- *PRESSURE* Pressure in Jet.
- RHO Mass density of jet.
- U Velocity of jet.
- CFL CFL number.
- TEND Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation

4.5.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.5.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- To visualize the fluid density, expand the Scalar Data tab and click the check box for fluids/q_0.
- Click the check box for Display Contours.
- Use the mouse to rotate the image within the Visualization Results pane.
- Drag the slider at the bottom of the visualization window to move through the simulation in time. The mass density distribution at the end of the simulation is shown in Fig. 4.5.

Note that q_0 is mass density, q_1 , q_2 , and q_3 are the three components of momentum density, and q_4 is energy density.

4.5.6 Further experiments

• Set U to 100.0 and increase TEND by a factor of 10 to see the effect of mach number on jet expansion.

4.6 Two-Fluid Magnetic Reconnection (gemChallenge.pre)

Keywords:

GEM Challenge, fast reconnection, two-fluid, hall effect, electron inertia, electromagnetic

4.6.1 Problem description

This problem shows fast magnetic reconnection based on initial conditions from the GEM challenge magnetic reconnection problem. The model used is fully electromagnetic, two-fluid with semi-implicit time stepping to step over the plasma and cyclotron frequency. This approach shows significant speedup for problems where the cyclotron or plasma frequency dominates the time step.

4.6.2 Creating the run space

The Two-Fluid Magnetic Reconnection example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Two-Fluid Magnetic Reconnection and press the Choose button.



Fig. 4.5: Visualization of the density in the Gas Injection Example as a color contour plot

- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.6.3 Input file features

In the standard GEM challenge problem the initial conditions are set up in non-dimensional form. In this case we mimic this scenario by setting coefficients such as ion charge and permeability to 1.0 and then ensure that the ion thermal velocity is approximately 0.01c. A realistic electron to proton mass ratio is maintained. Divergence cleaning for the magnetic field is performed using the hyperbolic approach and Poisson equation is preserved using electric field diffusion.

In this simulation reconnected magnetic flux is stored using a dynVector. The reconnected flux is then one-half the integral of the absolute value of By along y=0. This reconnected flux can be compared with published results, though it will typically only converge to those results at high resolution. If possible, increase the resolution and run the simulation in parallel.

The key variables of the input file are exposed in the "Setup" window. These variables allow one to set the following fields

- CFL CFL condition for the simulation
- *TEND* Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation
- *SPECIES_CHARGE* Charge of the positive species.
- ION_MASS Mass of the ion.
- ELECTRON_MASS Mass of the electron.
- GAS_GAMMA Specific heat ratio of the electron and ion fluid
- N0 The peak ion number density
- LAMBDA The current layer thicknesss
- B0 The X magnetic field at infinity
- PERTURBATION_FACTOR The factor that B0 is multiplied by to define the size of the perturbation
- *SPEED_OF_LIGHT* Speed of light
- EPSILON0 Permeability of free space
- *BP* Magnetic correction potential field divergence correction speed factor. The correction speed is given by speed=BP*c so the value BP should be near 1.0.
- *FLUID_NUMERICAL_FLUX* specifies the Riemann solver used to calculate an upwind approximation to the flux tensor. For hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, hlleEulerFlux. For magneto-hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, fWaveFlux. For more general systems, options include localLaxFlux, hlleFlux, fWaveFlux.
- *EM_NUMERICAL_FLUX* specifies the Riemann solver used to calculate an upwind approximation to the flux tensor. For hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, hlleEulerFlux. For magnetohydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, fWaveFlux. For more general systems, options include localLaxFlux, hlleFlux, fWaveFlux.
- *TIME_ORDER=first, second, third, fourth* sets the order of accuracy for the time-integration.

- *LIMITER=muscl,minmod,none* specifices the spatial limiting method used in reconstructing primary variables to use to ensure that method remains total value diminishing (TVD).
- *NX* Number of cells in the x direction
- NY Number of cells in the y direction
- *NZ* Number of cells in the z direction (3D only)
- X_MIN lower X position of grid
- X_MAX upper X position of grid
- *Y_MIN* lower Y position of grid
- Y_MAX upper Y position of grid
- Z_MIN lower Z position of grid (only in 3D)
- Z_MAX upper Z position of grid (only in 3D)

4.6.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.6.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- In the *Data View* dropdown menu, select *History*. The *history* field will provide you with access to dynVectors, in this case the reconnected flux. Plot 0 selects integratedFlux. The image below shows the result of a complete simulation Fig. 4.6.

4.6.6 Further experiments

- Decreasing the plasma layer thickness (LAMBDA) increases the initial reconnection rate.
- Decreasing the *SPECIES_CHARGE* reduces the magnetization (by increasing the Larmor radius of the electrons and ions) and prevents the magnetic field from maintaining equilibrium. Increasing the *SPECIES_CHARGE* does the opposite, the field is tied more closely to the plasma. Fast reconnection can occur in this case. However, it likely requires much higher resolution to effectively resolve the reconnection layer.

4.7 Magnetic Nozzle (magneticNozzle.pre)

Keywords:

Magnetic nozzle, Gas dynamic MHD



Fig. 4.6: Visualization of the integratedFlux history in the Two-Fluid Magnetic Reconnection example

4.7.1 Problem description

This example simulates the plasma acceleration in a magnetic nozzle used in micro vacuum arc thrusters to improve the performance. The magnetic field lines are generated using current coils placed around a cylinder. The magnetic field lines form a virtual nozzle for incoming plasma. Incoming plasma is generated from the arc discharge. The simulation is demonstrated using two dimensional domain though axi-symmetric is preferred. External magnetic field is generated using wire field equation. The flow is simulated using gasDynamicMhd equations(refer to USim reference manual). Arc is not simulated, instead constant number density, velocity, ionization number, and electron ion temperature ratio at the erosion surface are given as inputs.

This simulation can be performed with a USimHEDP license.

4.7.2 Creating the run space

The Magnetic Nozzle example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Magnetic Nozzle and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.7.3 Input file features

The following parameters can be varied to study different plasmas:

- GRIDFILE grid file name
- CFL CFL condition for the simulation
- ATOMIC_WEIGHT Atomic weight of ions
- ION_GAMMA Specific heat ratio ions
- *ELECTRON_GAMMA* Specific heat ratio of electrons
- N0 Initial number density of ions
- *ION_TEMP* Temperature of Ions at the nozzle inlet
- TEMPERATURE_RATIO Temperature ratio of electrons and ions at the nozzle inlet
- Z_RATIO Average change number of ions
- COIL_DIAMETER_RATIO Ratio of the diamter of current coil to the diamter of the thurster cylinder
- COIL_CURRENT Coil current to generate magnetic field
- V_IN Inlet velocity of the plasma x-component
- U_IN Inlet velocity of the plasma y-component
- INLET_NUMBER_DENSITY Number density of ions at the nozzle inlet
- RESISTIVITY Resistivity of plasma
- *TSTART* Simulation start time (seconds).
- *TEND* Simulation end time (seconds).
- *NUMDUMPS* Number of data dumps during the simulation

4.7.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.7.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/qMod_0 to visualize the ion density.

• Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The fluid density distribution at the end of the simulation is shown in Fig. 4.7.

Similarly other parameters such as magnetic field can be visualized. The description of output parameters follows

- E_0, E_1, E_2 electric field
- J_0, J_1, J_2 total current
- Z ionization number
- backgroundB_0, backgroundB_1, backgroundB_2 magnetic field induced by wire
- eta resistivity
- *nDens_0* number density of ions
- *nDens_1* number density of electrons
- *qMod_0* mass density of ions
- *qMod_1,qMod_2,qMod_3* momentum components
- *qMod_4* ion energy density
- qMod_5,qMod_6,qMod_7 magnetic field components
- *qMod_9* electron energy density



Fig. 4.7: Visualization of ion density for the Magnetic Nozzle example.

4.7.6 Further experiments

• Type of plasma can easily be changed by choosing the appropriate ATOMIC_WEIGHT.

- The effect of variation in arc current can be simulated by changing 'INLET_NUMBER_DENSITY' and/or V_IN. For example, increase the INLET_NUMBER_DENSITY and V_IN by 100%.
- The plasma jet focus can be adjusted by varying the *COIL_DIAMETER_RATIO* and *COIL_CURRENT*. Note that in this demo, the coil is actually a wire and coil diameter is distance between the wires. For instance, increase the *COIL_DIAMETER_RATIO* and/or *COIL_CURRENT* up to 100%.
- Try running in parallel on 2 cores by changing the grid to magneticNozzle2.msh

4.8 Merging Plasma Jets (plasmaJetMerging.pre)

Keywords:

Plasma Liner Experiment, plasma jet merging, radiation, fusion

4.8.1 Problem description

This problems shows plasma jet merging as investigated for the Los Alamos Plasma Liner Experiment by HyperV technologies. An ideal MHD model with general equation of state and bremsstrahlung radiation is used along with the plasma jet updater. By modifying the input file an arbitrary number of plasma jets can be included at arbitrary angles with respect to each other.

4.8.2 Creating the run space

The Merging Plasma Jets example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Merging Plasma Jets and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window as shown below. After any change is made, the *Save and Process Setup* button must be pressed again before a new run may commence.

4.8.3 Input file features

The following parameters can be modified to look at the effect on plasma jet merging:

- *DIM* Dimension of the simulation (2 or 3)
- *T_EV* Plasma temperature in electron volts
- NO Peak jet density in number per meter cubed
- AR Ion species atomic mass
- U Jet velocity towards the origin
- B0 Uniform initial magnetic field in the Z direction
- BX Uniform initial magnetic field in the X direction

- GAMMA Specific heat ratio of plasma
- *JET_INIT_LENGTH* Length of the region to initialize the jet.
- *JET_INIT_WIDTH* Width of the region to initialize the jet.
- *JET_DENSITY_FUNCTION* Function that hape of the jet as a function of parallel (x) and perpendicular (r) directions
- RAD Distance from the origin of the start of each plasma jet
- CFL CFL condition for the simulation
- TEND Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation
- PRESSURE_FACTOR Vacuum pressure factor which is the ratio of background pressure to peak initial pressure
- DENSITY_FACTOR Vacuum density factor which is the ratio of background density to peak initial density
- *CORRECTION_SPEED* Magnetic field divergence correction speed. Should be on the order of the fastest MHD wave speed in the simulation.
- *NUMERICAL_FLUX* specifies the Riemann solver used to calculate an upwind approximation to the flux tensor. For hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, hlleFlux. For magnetohydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, fWaveFlux. For more general systems, options include localLaxFlux, hlleFlux, fWaveFlux.
- TIME_ORDER first, second, third, fourth sets the order of accuracy for the time-integration.
- *LIMITER* muscl,minmod,none specifices the spatial limiting method used in reconstructing primary variables to use to ensure that method remains total value diminishing (TVD).
- NX Number of cells in the x direction
- *NY* Number of cells in the y direction
- *NZ* Number of cells in the z direction (3D only)
- *X_MIN* lower X position of grid
- *X_MAX* upper X position of grid
- *Y_MIN* lower Y position of grid
- *Y_MAX* upper Y position of grid
- Z_MIN lower Z position of grid (only in 3D)
- *Z_MAX* upper Z position of grid (only in 3D)

4.8.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.8.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/density to visualize fluid densities.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The fluid density distribution is early on in the simulation is shown in Fig. 4.8.



Fig. 4.8: Visualization of density in Merging Plasma Jets Merging example

4.8.6 Further experiments

- The default simulation has the background magnetic field set to 0. Set the background magnetic field B0=0.01 and run the simulation again. By visualizing q_7 in the visualization window you will be able to see the compression of the Z magnetic field from the incoming jets.
- We typically run these simulations with a background density factor of about 1×10^{-6} the initial peak density to simulate the vacuum. If this value is raised significantly by, for example, increasing DENSITY_FACTOR to 1×10^{-1} , you will see the jets plow into the background fluid, illustrating why it is important to maintain a low background density for these types of problems.

4.9 Ten-Moment, Two-Fluid Shock (tenMomentShock.pre)

Keywords:

Ten Moment Two-Fluid

4.9.1 Problem description

This example simulates a two-fluid shock where the ions use the 10 moment plasma model and the electrons use the 5 moment model.

This simulation can be performed with a USimHEDP license.

4.9.2 Creating the run space

The Ten-Moment, Two-Fluid Shock example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select Ten-Moment, Two-Fluid Shock and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.9.3 Input file features

The following parameters can be varied to study different plasmas:

- CFL used in the simulation
- SCALE scales the density and pressure keeping the temperature and acoustic speed constant
- NCELLS number of cells in the simulation
- TEND final simulation time
- NUMDUMPS number of data dumps during the simulation
- *XMAX* size of the domain

4.9.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.9.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- In the Data View dropdown menu, select 1-D Fields.
- The electron density shown in Fig. 4.9 can be visualized by clicking on *electrons_0* in *Plot 0*.

Similarly other parameters such as magnetic field can be visualized. The description of output parameters follows

- electrons_0 through electrons_4 the electron density, momentum density and energy density
- ions_0 through ions_9 the ion density, momentum density and 6 components of anisotropic energy density
- *em_0 through em_5* are the E and B fields

USimComposer – tenMomentShock.pre			
	Visualization Controls		Visualization Results
	Data View: 1 D Fields		fluids/electrons_0
Welcome		•	FFT Log Scale Zoom Navigate Save Image Labels Limits Reset View
=	Select up to 3 plots		
Setup	Plot 0		
	fluids/electrons_0 ‡		
Run	Location:	Window 1 ‡	
	Color:	Red \$	
Visualize Piero	Style:	Solid ‡	
			fluids/ions_0
	Plot 1		FET Log Scale Zoom Navigate Save Image Labels Limits Reset View
	fluids/ions_0	÷	- 1.00 - 0.90 - 0.90 - 0.70 0.60 0.50
	Location:	Window 2 ‡	
	Color:	Blue \$	
	Style:	Solid ‡	
	Plot 2		
	fluids/em_0 ‡		
	Location:	Window 3 \$	4 0.010 0.020 0.030 0.040 0.050 0.060 0.070 0.080 0.090 fluids/em_0 FFT Log Scale Zoom Navigate Save Image Labels Limits Reset View 9 1.0 1.0 1.0 1.0 1.0
	Color:	Green \$	
	Style:	Solid ‡	
	Plot 3		
	<none> +</none>		
	Location:	Window 4 ‡	
	Color:	Black ‡	
	Style:	Solid \$	
	Annotation Level:	Axes & Legends \$	Dump: 10 Step: 6000 Time: 1e-08
		Reload Data	0 10

Fig. 4.9: Visualization of electron mass density for the Ten-Moment, Two-Fluid Shock example.

4.9.6 Further experiments

1. Increase *XMAX* and *TEND* by the same factor to see how the solution evolves. Unlike the Euler equations and ideal MHD, the solution is not invariant with the scale of the system.

4.10 Verify EOS Table (verifyEOSTable.pre)

Keywords:

Equation-of-state table

4.10.1 Problem description

This example verifies the result of interpolation and inverse interpolation from a SESAME equation-of-state (EOS) table. Fake data is provided for the purpose of this example. To use this example with the PROPACEOS reader, simply set **INPUTFORMAT** to 1. This replaces instances of refmanual-sesameVariables with refmanual-propaceosVariables and replaces **301energy** and **301pressure** with **Eint** and **Ptot** in the operations strings, respectively.

In this example, a logarithmic grid is configured that provides the initial values for temperature and density. The energy and pressure tables are evaluated and subsequently inverse operations are applied to recompute the density and temperature. There are four inverse operations, two for each of the energy and pressure tables. The relative difference of the inverse and initial densities and temperature are computed and should be accurate to machine precision in regions of interest.

This test can be performed with a USimHEDP license.

4.10.2 Creating the run space

The verify EOS Table example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHEDP: High Energy Density Plasmas.
- Select *Verify EOS Table* and press the *Choose* button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

4.10.3 Input file features

The following parameters can be varied to verify different EOS tables:

- *TMIN* minimum temperature to check
- *TMAX* maximum temperature to check
- NMIN minimum mass density to check
- NMAX maximum mass density to check
- *EOSFILE* EOS table file name
- MATID Material ID required for SESAME only
- SPECIESMASS Species mass required for PROPACEOS only
- INPUTFORMAT Input format SESAME=0, PROPACEOS=1

4.10.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

4.10.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Scalar Data* and click the check box for *fluids/relativeDifference_0* to visualize the relative difference between the initial density and density computed from the inverse of the pressure EOS table as shown in Fig. 4.10.
- Check the other *fluids/relativeDifference_X* quantities 1-3 which correspond to the density from the inverse of the energy EOS table and the temperature from the inverse of the pressure and energy EOS tables, respectively.

The description of output parameters follows:

- density initial density
- temperature initial temperature
- energy Energy computed from interpolation of the EOS table
- pressure Pressure computed from interpolation of the EOS table
- densityFromPressure Density computed through inverse interpolation of the EOS pressure table
- densityFromEnergy Density computed through inverse interpolation of the EOS energy table
- temperatureFromPressure Temperature computed through inverse interpolation of the EOS pressure table
- temperatureFromEnergy Temperature computed through inverse interpolation of the EOS energy table
- *relativeDifference* Quantities correspond to the relative difference of the initial and density from the inverse of the pressure and energy EOS tables and the temperature from the inverse of the pressure and energy EOS tables, respectively.

4.10.6 Further experiments

- Change the material ID to check different materials
- Change the input file name to check different files
- When tables are not monotonic functions of density and temperature, note that incorrect results are expected. Ensure that the region of interest for computation produces valid results for the respective inverse operations that are used.



Fig. 4.10: Visualization of the relative difference between the initial density and density computed from the inverse of the pressure EOS table.

CHAPTER

USIMHS EXAMPLES

The USimHS examples illustrate how to solve problems for hypersonic flight. The USimHS examples can be executed with a USimHS license.

5.1 Diffusion (diffusion.pre)

Keywords:

diffusion, conduction

5.1.1 Problem description

This example models thermal diffusion from a cylindrical wall held at constant temperature. The diffusion scheme here can be used for all types of diffusion including thermal and species diffusion. This example uses the super time stepping integrator which accelerates the solution of diffusion type systems compared to standard explicit approaches.

This simulation can be performed with USimHS and USimHEDP license.

5.1.2 Creating the run space

The Diffusion example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select *Diffusion* and press the *Choose* button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.1.3 Input file features

The input folder has externally generate mesh file using *Gmsh*. The following parameters can be varied to simulate different flow regimes.

• GRIDFILE - Name of grid file

- NUMDUMPS Number of data dumps during the simulation
- EXPLICIT_CFL the explicit CFL to use to compute the number of STS cycles
- *STS_CFL* the actual CFL
- USESTS is 1 if the STS method is used 0 if the standard explicit approach should be used

5.1.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.1.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for fluids/q to get the temperature distribution.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The temperature distribution at the end of the simulation is shown in Fig. 5.1.

5.1.6 Further experiments

- Switch USESTS to 0 to see how much slower the simulation runs when standard explicit methods are used.
- Increase STS_CFL to see how the solution changes as larger and larger time steps are used.

5.2 Turbulent Flow Over Flat Plate (flatPlate.pre)

Keywords:

hydrodynamics, turbulence, Reynolds-Average Navier Stokes models

5.2.1 Problem description

This problem demonstrates boundary layer formation for subsonic flow over a flat plate, based on the problem described at http://turbmodels.larc.nasa.gov/flatplate.html. Two choices of Reynolds-Averaged Navier Stokes turbulence models are available: the Chien kEpsilon model described at http://turbmodels.larc.nasa.gov/ke-chien.html and the kOmega SST model described at http://turbmodels.larc.nasa.gov/sst.html.

This simulation can be performed with a USimHS license.



Fig. 5.1: Visualization of thermal diffusion.

5.2.2 Creating the run space

The Flat Plate example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select *Flow over Flat Plate* and press the *Choose* button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.2.3 Input file features

The input file allows the user to set a variety of problem parameters related to the physics, initial conditions, domain and solver used for boundary layer formation for subsonic flow over a flat plate.

The following parameters control the simulation physics:

- USE_KEPSILON = True, False selects whether to evolve the problem using the Chien kEpsilon model (USE_KEPSILON = True) or the kOmega SST model (USE_KEPSILON = False).
- *MACH_NUM* sets the ratio of the flow velocity to the sound speed (the Mach number).
- *T_ATM* sets the flow temperature in Kelvin.
- *P_ATM* sets the flow pressure in Pascals.
- TURBULENT_INTENSITY sets the intensity of turbulent fluctuations captured by RANS Model.
- *TURBULENT_REYNOLDS_NUMBER* is a dimensionless parameter describing ratio of turbulent viscosity to characteristic length scale.
- GAS_GAMMA sets the adiabatic index (ratio of specific heats) of the fluid.

The following parameters control the dimensionality, domain size and resolution of the simulation:

- VERTICAL_ZONES sets the number of zones in the direction perpendicular to the flow.
- VERTICAL_SIZE sets the size of the domain in the direction perpendicular to the flow.

The following parameters the length of the simulation and data output:

- *TEND* sets the end time for the simulation.
- *NUMDUMPS* sets the number of data dumps during the simulation
- WRITE_RESTART = False, True tells USim to output data necessary to restart the simulation. If this parameter is set to False then the Restart at Dump Number functionality in the Standard tab under Runtime Options in the Run window will not be available.

The following parameters control the USim solvers used to evolve the problem:

- *HYPERBOLIC_TIME_ORDER = first, second, third, fourth -* sets the order of accuracy for the hyperbolic system time-integrator.
- *DIFFUSION_TIME_ORDER = first, second* sets the order of accuracy for the diffusion system time-integrator.
- *DEBUG* = *False*,*True* sets whether to output data for debugging a run. Warning: this will output A LOT of information!

5.2.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.2.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize button in the left column of buttons.
- Press the "Open" button to begin visualizing.
- To visualize the fluid density, expand the Scalar Data tab and click the check box for fluids/velocity.
- Drag the slider at the bottom of the visualization window to move through the simulation in time. The velocity distribution at the end of the simulation is shown in Fig. 5.2.



Fig. 5.2: Visualization of the flow velocity flow over a flat plate as a color contour plot.

5.2.6 Further experiments

• Set USE_KEPSILON to False to use the KOmega SST RANS turbulence model.

• Increase VERTICAL_ZONES to study convergence of the boundary layer properties.

5.3 Flow over a Cylindrical Rod (highSpeedRod.pre)

Keywords:

Cylindrical Rod at Sea Level, hypersonic flow, Reactive flow, highSpeedRod

5.3.1 Problem description

This problem demonstrates aerothermal heating of a cylindrical body moving at Mach 23. The air surrounding the shock regions dissociates and ionizes. This simulation considers 7 species air chemistry model and simulates the flow at sea level. Viscous and conductive terms appropriate for a Sutherland viscosity model are implemented and are accelerated using Super Time Stepping techniques.

This simulation can be performed with a USimHS license.

5.3.2 Creating the run space

The Flow over a Cylindrical Rod example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select Flow over a Cylindrical Rod and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.3.3 Input file features

The input file allows the user to set problem parameters. They are:

- FREESTREAM_DENSITY free stream density
- FREESTREAM_TEMPERATURE free stream temperature
- *MACH_NUM* flow mach number
- NUMDUMPS number of data dumps during the simulation
- GRIDFILE mesh file for the simulation

The default choices for the free stream density and temperature are appropriate for sea level.

5.3.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.3.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for *fluids/qSpecies_6* to get the number density of the electrons.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The results at the end of the simulation is shown in Fig. 5.3.

The following parameters can also be visualized.

- cond Thermal conductivity
- pressure averagepressure of the mixture
- *qSpecies_0 qSpecies_6* number densities of the electrons
- q_0 mass density
- *q_1,q_2,q_3* momentum components
- *q_4* energy density
- temperature average temperature of the mixture
- velocity_0, velocity_1, velocity_2 three components of velocity
- visc Fluid (Sutherland) viscosity

Species indices are 0 to 6 (N2,N,O2,O,NO,NO+,e).

5.3.6 Further experiments

Four Gmsh fomat mesh files are included with this example, the default (*highSpeedRod.msh*), which is a low-resolution mesh that is partitioned for serial execution, versions of this mesh that is partioned so that it can be run with 2 (*highSpeedRod2.msh*), 4 (*highSpeedRod4.msh*) or 8 (('*highSpeedRod8.msh*) cores along with a high resolution mesh that is partioned for either two (*highSpeedRod4.msh*) or 24 (*highSpeedRod4.msh*) or 24 (*highSpeedRod4.msh*) cores. To run the example using this moderate resolution mesh on 2 cores, proceed as follows:

- Return to the "Setup" window by pressing the Setup button in the left column of buttons.
- Enter the mesh file name *highSpeedRod2.msh* next to *meshFile*.
- Press the Save And Process Setup button in the upper right corner.
- Proceed to the run window as instructed by pressing the Run button in the left column of buttons.
- In the "Run" window, press the MPI button in the left pane.



Fig. 5.3: Visualization of the electrons density for the Flow over a Cylindrical Rod example
- USimComposer highSpeedRod.pr Logs and Ou Runtime Options Parallel Execution Option: Run Force Stop Run with MPI Log File Browser Number of Cores 2 I. Finalizing updater 'init Finalizing updater 'initNonKineticEnergy' Finalizing updater 'initSpecies' Finalizing updater 'initTemperature Finalizing updater 'nanChecker' Finalizing updater 'rkUpdater' Finalizing updater 'setViscSource' Finalizing updater 'sourceUpdater' Finalizing updater 'speciesCorrector' ? Finalizing updater 'stsUpdater' Finalizing updater 'temperatureCorrector' Finalizing updater 'timeStepRestriction' Finalizing updater 'updateInitialEnergy Finalizing component 'fluids' Engine completed successfully -Analysis Step-Running in directory /Users/angle/Documents/txcorp/USimComposer1.0/runs/highS peedRod Analysis step launched successfully Executing analysis script: /Applications/USimComposer.app/Contents/scripts/genhist.py Searching for Dyn Vector data in: cond Searching for Dyn Vector data in: pressure Searching for Dyn Vector data in: g Searching for Dyn Vector data in: qSpecies Searching for Dyn Vector data in: temperature Searching for Dyn Vector data in: velocity Searching for Dyn Vector data in: visc No Dyn Vectors found, thus no Histories will be generated Engine completed successfully To see results, click on the "Visualize" icon in the icon panel. Reset Options
- Check the box marked Run with MPI and set Number of Cores equal to 2 as pictured in Fig. 5.4.

Fig. 5.4: Run window showing the parallel option.

After setting the Number of Cores, run the simulation:

• To run the file, click on the *Run* button in the upper right corner. of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully."

After the simulation has executed, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize button in the left column of buttons.
- Press the "Open" button to begin visualizing.
- To visualize the geometry, expand the geometry tab and click the checkbox for *fluids/domain*.
- To visualize the electron density, expand the Scalar Data tab and click the check box for fluids/qSpecies_6.
- Drag the slider at the bottom of the visualization window to move through the simulation in time.

5.4 Supersonic Crossflow over a Cylinder (mach2Cylinder.pre)

Keywords:

Flow over cylinder, Supersonic, Navier-Stokes

5.4.1 Problem description

This simulation shows the supersonic flow over a cylinder. The formation of bow shock and the final steady wake can be seen in this laminar flow simulation. Full Navier-Stokes equations are used. Laminar flow assumption is used. Unstructured grid is used here. This grid was generated using gmsh. The convective and viscous parts are fully decoupled i.e the flow can be changed to inviscid by removing the viscous terms from the integration Updater. The properties of the fluid varying with temperature are computed within the input file. In this example, Sutherland's formulas are used to obtain viscosity and thermal conductivity. The specific heats are assumed constant. Note that, the grid used in demonstrating this example is way coarse to display initial vortex shedding.

This simulation can be performed using USimHS license.

5.4.2 Creating the run space

The Supersonic Crossflow over a Cylinder example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select Supersonic Crossflow over a Cylinder and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.4.3 Input file features

The following parameters can be varied:

- *CFL* CFL condition for the simulation
- ATOMIC_MASS Atomic mass of the gas
- GAS_GAMMA Specific heat ratio of the gas
- RHO0 Free stream density of the gas
- P0 Free stream pressure of the gas
- *U0* Free stream velocity of the gas x-component
- *V0* Free stream velocity of the gas y-component
- SURFACE_TEMP Surface temperature of the body
- CHARACTERISTIC_LENGTH Characteristic length of the body
- *MU_REF* Dynamic viscosity of the free stream gas
- SUTHERLAND Sutherland coefficient
- TEMP_REF Reference temperature in Sutherland's formula
- *TSTART* Simulation start time (seconds).
- TEND Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation

- GRIDFILE Name of grid file
- DECOMPOSE Type true for triangle and tetrahedral, false for 1d, quadrilateral and hexahedral
- CYLINDER_RADIUS Radius of the cylinder
- X_MIN Bottom left x-coordinate of the grid
- Y_MIN Bottom left y-coordinate of the grid
- X_MAX Top right x-coordinate of the grid
- *Y_MAX* Top right y-coordinate of the grid

Note that the input file comes with an externally generated unstructured mesh using *Gmsh*. The parameters *CYLIN-DER_RADIUS*, (*X_MIN*, *Y_MIN*), and (*X_MAX*, *Y_MAX*) can be changed to accommodate a new mesh generated using *Gmsh*. The cylinder's center is at origin.

5.4.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.4.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Geometries* in the *Visualization Controls* pane and click the checkbox for *fluids/domain* to visualize simulation geometry.
- Expand Scalar Data and click the check box for fluids/temperature to visualize the temperature distribution.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The final distribution is shown in Fig. 5.5.

The conservative parameters density, three components of momentum, and energy can also be visualized using q_0, q_1, \dots, q_5 respectively. *source_0 to source_3* represent the viscous sources of momentum and energy equations.

5.4.6 Further experiments

- Change the flow speed: For example increase U0 to 13600 (Mach 4) keeping the other flow parameters unchanged. Follow the steps and complete the simulation. The rise in shock temperature can be observed from the temperature distribution in the visualization window.
- Parallel: In the current version of USim, pre-partitioned unstructured mesh has to be used to run in parallel. The input file folder has partitioned mesh files for 2, 4, and 8 cores. (mach2CylinderQuad2.msh, mach2CylinderQuad4.msh, mach2CylinderQuad8.msh).



Fig. 5.5: Visualization of temperature distribution in the Supersonic Crossflow over a Cylinder example

5.5 Blunt-Body Reentry Vehicle (ramC.pre)

Keywords:

RAMC, hypersonic flow, reactive flow, mass injection, cylindrical, Navier-Stokes

5.5.1 Problem description

Reentry of RAMC-type module is simulated. The aerothermal heating due the formation of shock wave and the resulting weakly ionized plasma are simulated at an altitude of 61 km. Navier-Stokes equations are used for flow simulation. Thermophysical properties of air are computed internally using kinetic theory. This simulation is carried out for zero angle of attack and hence axi-symmetric form of equations are used. 7 species air chemistry model is used to obtain the species densities. Given distribution of temperature along with mass injection can be specified on the surface. Na, Ca, and K are injected. Ca and Na are injected in the nose cap region. K and Na are injected from the lateral surface. This simulation considers 10 species in total.

This simulation can be performed with USimHS license.

5.5.2 Creating the run space

The ramC example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select *ramC* and press the *Choose* button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.5.3 Input file features

The input folder has externally generate mesh file using *Cubit*. The following parameters can be varied to simulate different flow regimes.

- *TSTART* Simulation start time (seconds).
- *TEND* Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation
- GRIDFILE name of grid file
- REACTIONS_ATOMIC_DATA name of the file containing reactions and atomic data
- W0 z-component of free stream velocity
- FREESTREAM_DENSITY free stream density
- FREESTREAM_TEMPERATURE free stream temperature
- *SURFACE_TEMPERATURE* surface temperature
- *INJECTION_DENSITY1* density at injection boundary1

- INJECTION_VELOCITY1 X component velocity at injection boundary1
- *MWinj1_1* molecular weight of species 1
- *MWinj1_2* molecular weight of species 2
- *MFinj1_1* mass fraction of species 1
- *MFinj1_2* mass fraction of species 2
- INJECTION_DENSITY2 density at injection boundary2
- INJECTION_VELOCITY2 X component velocity at injection boundary2
- MWinj2_1 molecular weight of species 1
- *MWinj2_2* molecular weight of species 2
- *MFinj2_1* mass fraction of species 1
- *MFinj2_2* mass fraction of species 2
- *NUMERICAL_FLUX* specifies the Riemann solver used to calculate an upwind approximation to the flux tensor. For hydrodynamic problems, options include localLaxFlux, hlleFlux, hlleFlux, hlleFlux. For magnetohydrodynamic problems, options include localLaxFlux, hlleFlux, hlldMhdFlux, fWaveFlux. For more general systems, options include localLaxFlux, hlleFlux, fWaveFlux.
- TIME_ORDER=first, second, third, fourth sets the order of accuracy for the time-integration.
- CFL_CONVECTIVE CFL condition number for convective terms
- *VISCOUS_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on kinematic viscosity
- *THERMAL_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on thermal diffusicity
- BASEMENT_TEMPERATURE least possible temperature in the domain (K).

Note: More information about the format of the file containing the reactions and atomic data can be found in the reference manual at refmanual-SpeciesDataFile.

5.5.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the Run window as instructed by pressing the Run icon in the workflow panel.
- To run the simulation, click on the Run button in the upper right corner of the Logs and Output Files pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.5.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for *fluids/q_0* to visualize the density distribution.

• Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The fluid density distribution at the end of the simulation is shown in Fig. 5.6.

The following parameters can also be visualized:

- *a* speed of sound
- *mwAvg* average molecular weight of gas mixture (molecular weight varies due to the change in composition of gas)
- cpR_0 cpR_9 constant pressure specific heat of species
- cpAvg average specific heat of fluid
- gammaAvg specific heat ratio of fluid
- *p* total pressure
- pe electron pressure
- ph heavy particle pressure
- q_0 mass density
- *q_1,q_2,q_3* momentum components
- *q_4* energy density
- speciesDens_0 speciesDens_9 number densities of the species
- temperature average temperature of the mixture
- *velocity_0,velocity_1,velocity_2* three components of velocity

Species indices are 0 to 6 (N2,N,O2,O,NO,NO+,e,Ca,Na,K).

5.5.6 Further experiments

- The freestream velocity *W0* may be changed to simulate different Mach numbers at a given altitude. Increase in electron density as a result of increased aerothermal heating can be noticed.
- The freestream temperature and density can be changed to simulate the changes in altitude. Lets say at 50 km altitude, the density and temperature of air are 0.000978 kg/m^3 and 270 K. Simulation without changing the freestream air speed shows that the electron density increases mainly due to the increase in freestream density.
- Change the surface temperature, mass injection densities and velocities. The injection species may also be changed by changing their atomic properties both in the input file and *air7SpeciesAb.txt* file.

5.6 3D Reentry Vehicle (ramC3d.pre)

Keywords:

hypersonic, Navier-Stokes, ballistic, reentry, reactions, ablation

5.6.1 Problem description

This example simulates the ballistic reentry of the RAMC module. The simulation is performed at an altitude of 61 km and an angle of attack of 15° . The surface of RAMC is assumed to be made up of carbon material. Standard radiation equilibrium model is used to compute the surface temperature and then ablation of carbon from the surface



Fig. 5.6: Visualization of density distribution for the Blunt-Body Reentry Vehicle example.

is obtained. The fluid contains 7 air species and carbon atoms. The reactions and atomic data are given in the external text data file air7SpeciesAbCarbon.txt. Grid is generated using cubit.

This simulation can be performed using USimHS license.

5.6.2 Creating the run space

The 3D Reentry Vehicle example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template dialog, expand USimHS: Hypersonics.
- Select 3D Reentry Vehicle and press the Choose button.
- In the *Choose a name for the new runspace* dialog, press the *Save* button to create a copy of this example in your run area.
- Press the Save And Process Setup button in the upper right corner of the Editor pane.

The basic example variables are editable in the *Editor* pane of the *Setup* window. After any change is made, the *Save* and *Process Setup* button must be pressed again before a new run commences.

5.6.3 Input file features

The following parameters can be varied:

- GRIDFILE name of grid file
- TEND Simulation end time (seconds).
- NUMDUMPS Number of data dumps during the simulation
- REACTIONS_ATOMIC_DATA name of the file containing reactions and atomic data
- SPEED free stream velocity
- AOA angle of attack
- FREESTREAM_DENSITY free stream density
- FREESTREAM_TEMPERATURE free stream temperature
- SURFACE_EMISSIVITY emissivity of the surface
- GAS_EMISSIVITY emissivity of the hot gas in the vicinity of surface
- MW1_1 molecular weight of species 1
- ABP01_1 reference pressure of species 1
- *ABDH1_1* evaporation enthalpy of species 1
- *ABT01_1* reference temperature of species 1
- CFL_CONVECTIVE CFL condition number for convective terms
- *VISCOUS_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on kinematic viscosity
- *THERMAL_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on thermal diffusicity
- BASEMENT_TEMPERATURE least possible temperature in the domain (K).

The speed, angle of attack, free stream density, temperature are 7650 m/s, 15° , $2.816^{-4}kg/m^3$, and 244.3 K respectively. Surface material is carbon. Note that the input file comes with an externally generated unstructured mesh using *cubit*.

Note: More information about the format of the file containing the reactions and atomic data can be found in the reference manual at refmanual-SpeciesDataFile.

5.6.4 Running the simulation

After performing the above actions, continue as follows:

- Proceed to the *Run* window as instructed by pressing the *Run* icon in the workflow panel.
- To run the simulation, click on the *Run* button in the upper right corner of the *Logs and Output Files* pane.

You will also see the engine log output in the *Logs and Output Files* pane. The run has completed when you see the output, "Engine completed successfully."

5.6.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand Scalar Data and click the check box for *fluids/speciesDens_7*.
- Check the *Clip All Plots* box and set the Z-intercept to 0.
- Drag the slider at the bottom of the *Visualization Results* pane to move through the simulation in time. The distribution at the end of the simulation is shown in Fig. **??**.

The conservative parameters density, three components of momentum, and energy can also be visualized using $q_0, q_1, .., q_5$ respectively.

5.6.6 Further experiments

- Change the flow speed: For example, decrease *SPEED* to 6000, keeping the other flow parameters unchanged. Follow the steps and complete the simulation.
- AOA: angle of attack may be changed to simulate trajectory maneuver.
- Altitude: Change in altitude can be simulated by varying the freestream density and temperature.
- Material: Change the surface material to say aluminum. The properties of aluminum $MW1_1 = 27.0$, $ABP01_1 = 0.133$, $ABDH1_1 = 304807.868$, $ABT01_1 = 1351.9932$. The name of the species in the *reactionTableRhs* block has to be updated to *Al* in the .pre file. In addition to these, the molecular weight and molecular diameter of species 7 have to be changed in the air7SpeciesAbCarbon.txt file. The change is given below:

MOLECULARWEIGHT START SPECIES N2 N O2 O NO NO_p1 e Al 28.0 14.0 32.0 16.0 30.0 30.0 5.5e-4 27.0 MOLECULARWEIGHT END MOLECULARDIA START



Fig. 5.7: Ablation species density on RAMC during reentry

SPECIES N2 N O2 O NO NO_p1 e Al 2.5e-10 2.0e-10 5.0e-10 2.0e-10 2.5e-10 2.5e-10 5.0e-13 2.7e-10 MOLECULARDIA END

• Parallel: carry out the simulation on 2, 4, or 8 cores using the *MPI* options.

CHAPTER

COUPLED USIMHS AND USIMHEDP EXAMPLES

These examples illustrate how to solve problems for hypersonic flight where plasma effects are important. These examples require both a USimHEDP and a USimHS license for execution.

6.1 Arc Plasma Torch (plasmaTorch.pre)

Keywords:

plasma, DC arc

6.1.1 Problem description

This example simulates the arc plasma torch. The simulation includes the formation of a DC arc, ionization of working gas and expansion through the torch. An axisymmetric domain is utilized for a faster demonstration of the simulation. Argon gas is the working gas and first ions and electrons are considered. The Navier-Stokes equations are solved for the overall fluid transport. Individual continuity equations are equations are solved for the species transport. Electron impact ionization is considered. The rate constants and atomic data, required for the estimation of transport properties, is provided in the text file *argon.txt*. Turbulence is included in this simulation using Cheien kEpsilon model described at http://turbmodels.larc.nasa.gov/ke-chien.html.

This simulation requires both a USimHS and USIMHEDP license.

6.1.2 Creating the run space

The Arc Plasma Torch example is accessed from within USimComposer by the following actions:

- Select the New from Template menu item in the File menu.
- In the resulting New from Template window, expand USimHS.
- Select Arc Plasma Torch and press the Choose button.
- In the resulting dialog, press the Save button to create a copy of this example in your run area.

The basic variables of this problem should now be settable in text boxes in the right pane of the "Setup" window.

6.1.3 Input file features

The following parameters can be varied:

• *GENERATE_ARC* - option to start and stop the arc (1 or 0)

- SLPM Flow rate (standard liter per minute)
- INLET_TEMPERATURE Fluid temperature at the inlet (K)
- *MW* Molecular weight(number)
- REACTIONS_ATOMIC_DATA Name of the user specified file containing the reaction rates and atomic data
- MAXRATE Limit to the rate of change of species number density (1/(m^3 s))
- TOTALCURRENT Total current of the arc (A)
- INITIAL_ELECTRICAL_CONDUCTIVITY Initial value of electrical conductivity (S/m)
- TURBULENT_INTENSITY sets the intensity of turbulent fluctuations captured by RANS Model.
- NUMDUMPS Number of data dumps during the simulation
- *TEND* Simulation end time (seconds)

Note that the input file comes with an externally generated unstructured mesh using CUBIT.

6.1.4 Running the simulation

After performing the above actions, continue as follows:

This simulation is run in two steps. Arc is established in the first step and then fluid plasma propagation is solved in the second step. The default time is set to 60.0e-6 seconds. With the default parameters, it will take 60.0e-6 seconds to establish the arc. If the properties are changed, *TEND* has to be chosen appropriately to allow the arc to establish.

STEP-1:

- Press the Save And Process Setup button in the upper right corner.
- Proceed to the run window as instructed by pressing the Run button in the left column of buttons.
- To run the file, click on the *Run* button in the upper right corner. of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully."

STEP-2:

- In the editor window (with View Parameters on) turn off the arc by setting GENERATE_ARC = 0
- Increase the TEND to 200.0e-6. Increase the NUMDUMPS to 20. Save And Process Setup again.
- Proceed to the run window as instructed by pressing the Run button in the left column of buttons.
- Restart the simulation from STEP-1 by entering 1 in Restart at Dump Number available on the left-pane.
- Run the simulation as given in *STEP-1*.

6.1.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize button in the left column of buttons.
- Press the "Open" button to begin visualizing.
- On the left side of the window, click on fluids/avgTemp to view the average temperature as sown in Figure , Fig. 6.1.

J USimComposer - plasmaTorch.pre _ 🗆 🗙					
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Fig. 6.1: Arc plasma flow in the torch. Average temperature.

6.1.6 Further experiments

- Change the TOTALCURRENT.
- Change the INITIAL_ELECTRICAL_CONDUCTIVITY.
- Run the simulation on 2 and 8 cores using the MPI Runtime Option.

6.2 Radio Communication Blackout (ramCEM.pre)

Keywords:

hypersonic, reentry, plane-wave, blackout

6.2.1 Problem description

This example simulates the propagation of electro-magnetic wave through plasma. The objective is to simulate the communication blackout on re-entry vehicles. A plane sine wave is sent from the left hand side face of the domain. Maxwell's equations are then solved to get the electric and magnetic field components in the simulation domain.

This simulation requires both a USimHS and USIMHEDP license.

6.2.2 Creating the run space

The Radio Communication Blackout example is accessed from within USimComposer by the following actions:

• Select the *New from Template* menu item in the *File* menu.

- In the resulting New from Template window, expand USimHS or USimHEDP.
- Select Radio Communication Blackout and press the Choose button.
- In the resulting dialog, press the *Save* button to create a copy of this example in your run area.

The basic variables of this problem should now be settable in text boxes in the right pane of the "Setup" window.

6.2.3 Input file features

The following parameters can be varied:

- *TEND* Simulation end time (seconds)
- *EM_FREQUENCY* wave frequency
- EM_CYCLES number of EM wave cycles to evolve for
- NUMDUMPS Number of data dumps during the simulation
- GENERATE_INITIAL_CONDITION Generate the evolved plasma distribution on the mesh
- GRIDFILE name of grid file
- REACTIONS_ATOMIC_DATA name of the consisting of reactions and atomic data
- SPEED free stream velocity
- AOA angle of attack
- FREESTREAM_DENSITY free stream density
- FREESTREAM_TEMPERATURE free stream temperature
- SURFACE_EMISSIVITY emissivity of the surface
- GAS_EMISSIVITY emissivity of the hot gas in the vicinity of surface
- *MW1_1* molecular weight of species 1
- ABP01_1 reference pressure of species 1
- *ABDH1_1* evaporation enthalpy of species 1
- *ABT01_1* reference temperature of species 1
- CFL_CONVECTIVE CFL condition number for convective terms
- *VISCOUS_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on kinematic viscosity
- *THERMAL_DIFF_TIMESTEP_FACTOR* Factor to further decrease the internally computed time step based on thermal diffusicity
- BASEMENT_TEMPERATURE least possible temperature in the domain (K)

Note that the input file comes with an externally generated unstructured mesh using cubit.

6.2.4 Running the simulation

This example simulates the propagation of an EM wave through the plasma layer surrounding the re-entry vehicle. The first step in the simulation is to generate this plasma distribution, accomplished by setting *GENER*- $ATE_INITIAL_CONDITION = True$ (the default). With this choice, generate the plasma distribution by proceeding as follows:

- Press the Save And Process Setup button in the upper right corner.
- Proceed to the run window as instructed by pressing the Run button in the left column of buttons.
- To run the file, click on the *Run* button in the upper right corner. of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully."

Once the simulation has completed, return to the "Setup" window and set *GENERATE_INITIAL_CONDITION = False* and increase the *NUMDUMPS* to 20. Then:

- Press the Save And Process Setup button in the upper right corner.
- Proceed to the run window as instructed by pressing the Run button in the left column of buttons.
- Chose the restart dump number equal to the final dump file from the previous run.
- To run the file, click on the *Run* button in the upper right corner. of the window. You will see the output of the run in the right pane. The run has completed when you see the output, "Engine completed successfully."

6.2.5 Visualizing the results

After performing the above actions, continue as follows:

- Proceed to the Visualize window as instructed by pressing the Visualize icon in the workflow panel.
- Press the Open button to begin visualizing.
- Expand *Scalar Data* and click the check box for *fluids/em_1* to visualize the y-component of electric field as shown in Figure 6.2. Refer to refmanual-maxwellEqn to see the definitions of remaining components.



Fig. 6.2: Plane EM wave propagation through plasma layer on RAMC during re-entry.

6.2.6 Further experiments

- Change the wave frequency.
- Run the simulation without plasma. Do not use the restart option and make TEND = 0 and *GENER*-*ATE_INITIAL_CONDITION* = *False*.
- Parallel: carry out the simulation on 2 and 8 cores using the MPI option.

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