TFAWS AUGUST 2003
VULCAN CFD CODE OVERVIEW / DEMO

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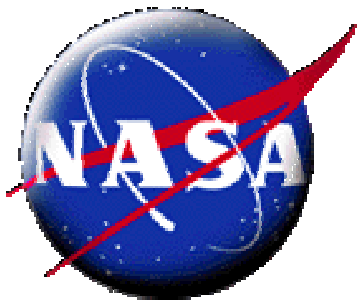


Hypersonic Airbreathing Propulsion Branch

VULCAN DEVELOPMENT HISTORY

- Evolved from the LARCK code development project (1993-1996).
  - LARCK developed as a cell-centered, finite volume, multi-block multi-grid, code to solve the full Navier-Stokes equations for turbulent non-equilibrium chemically reacting flows to replace SPARK.
  - Assumed PDF turbulent chemistry models developed and added.
- VULCAN was created from LARCK as part of a RAM/SCRAMJET CFD code development project conducted under contract to the Air Force Research Lab, Propulsion Directorate, at Wright Patterson Air Force Base (1996-1997).
  - Multi-region domain decomposition paradigm added.
  - Space Marching scheme added.
  - Wall matching (wall functions) added.
- VULCAN code and algorithm development continued by Hypersonic Airbreathing propulsion branch (1997-2003).
  - Space marching with multi-grid and sub-stepping developed.
  - Turbulent model options expanded (Wilcox, EARS, etc.).
  - Graphical User interfaces developed.
  - Parallel processing version (MPI) developed.
  - Non-C(0) block-to-block interface capability added.
  - LES scheme added by AFRL WPAFB.
  - New chemical kinetic and turbulent chemistry models added.

GOVERNING EQUATIONS AND SOLUTION METHODS

- Solve the equations governing 2-D, axisymmetric or 3-D calorically perfect or thermally perfect non-equilibrium chemically reacting flows.
    - Structured grid, cell centered, finite volume, density based method.
    - Inviscid fluxes computed to 2nd order accuracy using vanLeer's MUSCL scheme with either of:
        - flux difference split scheme of Phil Roe, or the
        - low dissipation flux split scheme of Jack Edwards
    - Viscous fluxes computed to 2nd order accuracy using either a
        - thin layer gradient construction (ignores cross derivatives)
        - full gradient construction (includes cross derivatives)
- Solve the full spatially elliptic Euler or full Navier-Stokes equations by integrating the conservative form of the unsteady equations in real or psuedo-time.
- Solve the spatially hyperbolic Euler or parabolized Navier-Stokes equations by integrating the conservative form of the unsteady equations in psuedo-time.

DOMAIN DECOMPOSITION METHODOLOGY

- Four level hierarchy of domain decomposition.
  - Structured grid cell : a six sided finite volume.
  - Structured grid block : an Imax X Jmax X Kmax group of cells.
  - Structured grid region : a group of blocks solved together.
  - Structured grid computational domain : Sum of all cells, blocks and regions.

- The no. of governing equations is consistent across all cells in the computational domain.

- The no. and order of the chemical species is consistent across all cells in the computational domain.

- The thermodynamic and transport models are consistent across all cells in the computational domain.

- Turbulence models can be turned on or off at the block level.

- Chemical reaction models can be turned on or off at the block level.

DOMAIN DECOMPOSITION METHODOLOGY

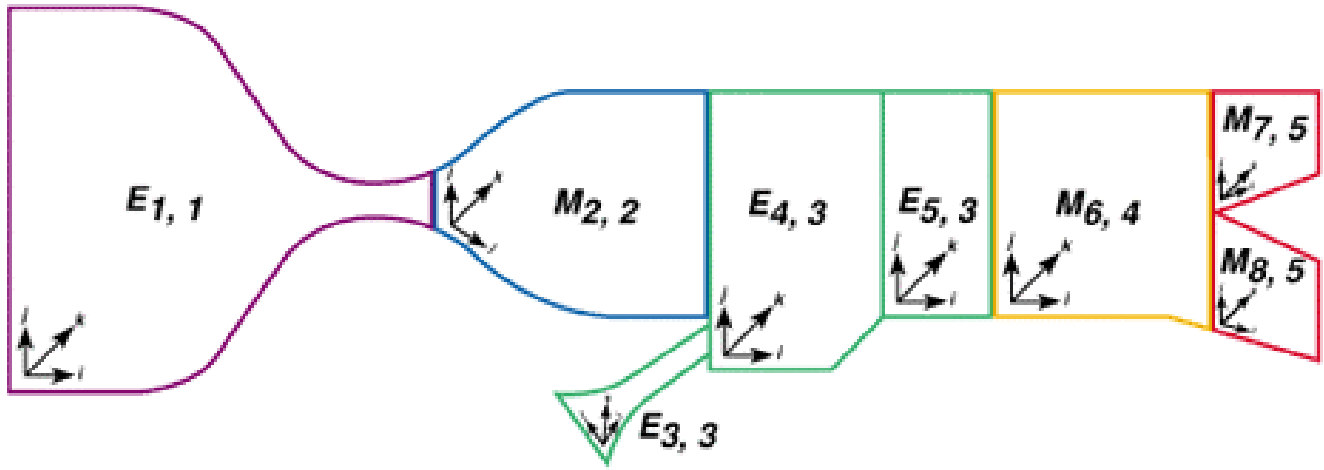
Computational domain decomposition rules

1- Block: A logical i, j, k group of grid nodes or cells

2- Region: A group of blocks solved simultaneously using a common algorithm;

a) Spatially elliptic: $E_{B,R}$; Solve block B in region R using an elliptic algorithm

b) Spatially marched: $M_{B,R}$; Solve block B in region R using a space marching algorithm



3- Regions are solved in ascending order

4- Marching blocks that connect across block i-faces MUST be in different regions

5- Marching blocks can be marched in the i-direction ONLY!

THERMODYNAMIC AND TRANSPORT MODELS

- Thermodynamic properties are modeled either as
  - Single component calorically perfect gas (constant C_p)
  - Arbitrary mixture of thermally perfect gases where
    - Curve fits of C_p, enthalpy, and Gibbs free energy are obtained from a species curve fit data base provides with VULCAN
    - Curve fits are provided for selected species using either
      - Single interval 7th order curve fit (300-6000 Kelvin range)
      - Two interval 7th order curve fit (300-6000 Kelvin range)
      - Three interval 9th order curve fit (200-20,000 Kelvin range)

- Transport properties (molecular viscosity, thermal conductivity) using
  - Sutherland's law for the molecular viscosity and constant Prandtl no. for the thermal conductivity of a single component calorically perfect gas.
  - Sutherland's law for species molecular viscosity with Wilke's law for the mixture molecular viscosity.
  - Sutherland's law for species molecular conductivity with Wassileja's for the mixture molecular conductivity.

CHEMICAL KINETIC MODELS

- Species production/destruction computed using law of mass action.
  - Reaction model data base provided where reactions are specified in equation form.
  - A 3 step - 6 specie ethylene mechanism would look like

    'C2H4 + O2 <=> 2CO + 2H2'
    '2CO + O2 <=> 2CO2'
    '2H2 + O2 <=> 2H2O'
    - Reaction equations can be specified as bi-directional

      'C2H4 + O2 <=> 2CO + 2H2'
    - and/or specified as uni-directional.

      'C2H4 + 2O2 => 2CO + 2H2O'
  - Forward chemical reaction coefficients are modeled using Arrhenius model.

    $$k_f = A\, T^B\, e^{(-Ta/T)}$$
  - Backward chemical reaction coefficients modeled using either an
    - Arrhenius model or an
    - equilibrium model $k_b = k_f / k_e$
  - Third body efficiencies are modeled / specified for each individual third body reaction.

- Global reaction rate models using an arbitrary reaction order method. **(NEW)**

MEAN FLOW TURBULENCE MODELS

Momentum and energy turbulence effects are modeled using two-equation turbulence models which solve for :

- Turbulent kinetic energy
- Dissipation related variable
    - dissipation rate of turbulent kinetic energy (epsilon) or
    - specific dissipation rate of turbulent kinetic energy (omega)

- The Reynolds stresses present in the mean flow equations and the production terms of the two-equation models are consistently modeled using either a
    - Boussinesq model or a
    - Explicit algebraic stress model (Gatski-Speziale).

- A new two-equation turbulent scalar diffusion model for thermal diffusion is currently under development through a NGLT grant. **(NEW)**

MEAN FLOW TWO-EQUATION TURBULENCE MODELS

- k-epsilon based models
  - Low Reynolds no. wall integration model of Abid.
  - Explicit algebraic Reynolds stress model of Gatski and Speziale.
- k-omega based models
  - Wilcox's 1998 family of models
    - High Reynolds no. wall integrable model
    - High Reynolds no. with wall matching functions
    - Low Reynolds no. wall integrable model
    - Explicit algebraic Reynolds stress wall integrable model
    - Explicit algebraic Reynolds stress with wall matching functions
  - Menter's family of models
    - Baseline high Reynolds no. wall integrable model
    - Baseline high Reynolds no. model with wall matching functions
    - Shear stress transport (SST) high Reynolds no. wall ntegrable model
    - Shear stress transport (SST) high Reynolds no. with wall matching functions

WILCOX WALL MATCHING FUNCTIONS

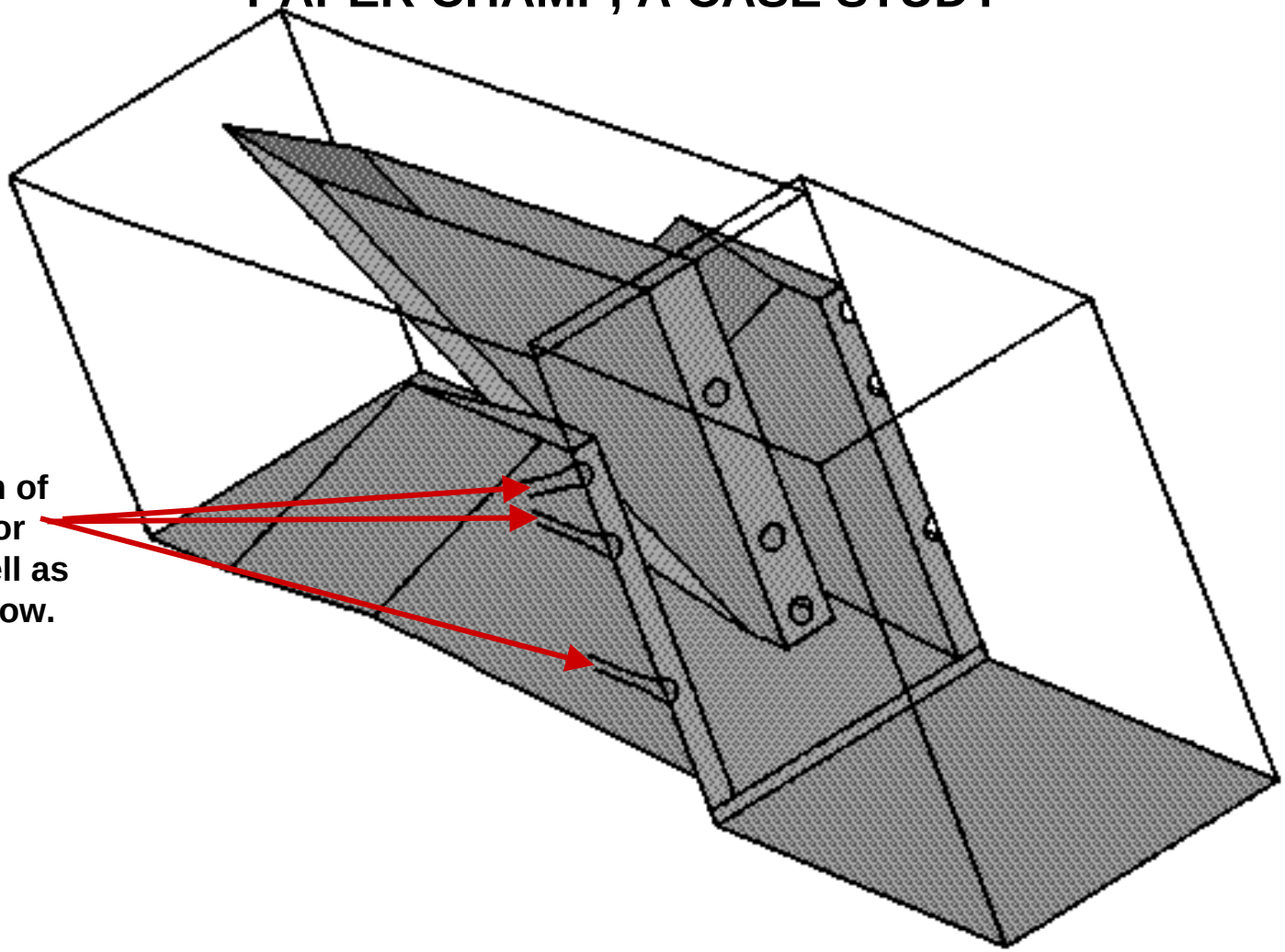
- Wall matching functions are:
  - Corrected for the streamwise pressure gradient effects.
  - Corrected for compressibility effects (vanDriest II).
  - Blended with the high Reynolds no. solve-to-wall method for y+<10.
  - Solved iteratively using Newton's method.

- Wall matching functions are solved to provide:
  - The wall shear stress magnitude.
  - The wall heat flux magnitude.
  - Solution to the k and omega equations at the first cell center off the wall.

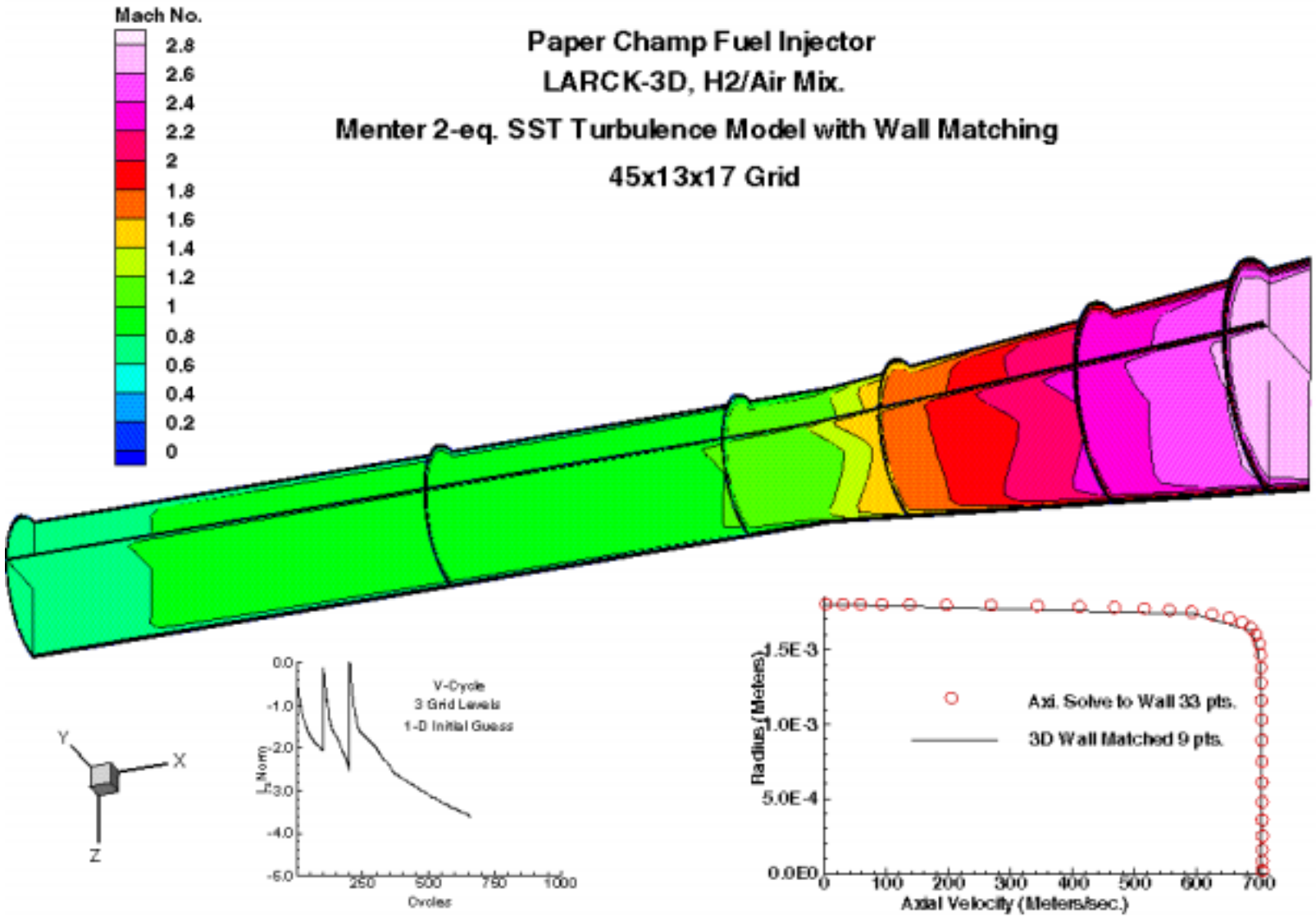
- Wall matching functions can be:
  - Used on the coarse and/or fine grids.
  - Used on any subset on a boundary face.
  - Mixed with with solve-to-wall boundary conditions.

FIDELITY OF WALL MATCHING FUNCTIONS: PAPER CHAMP, A CASE STUDY

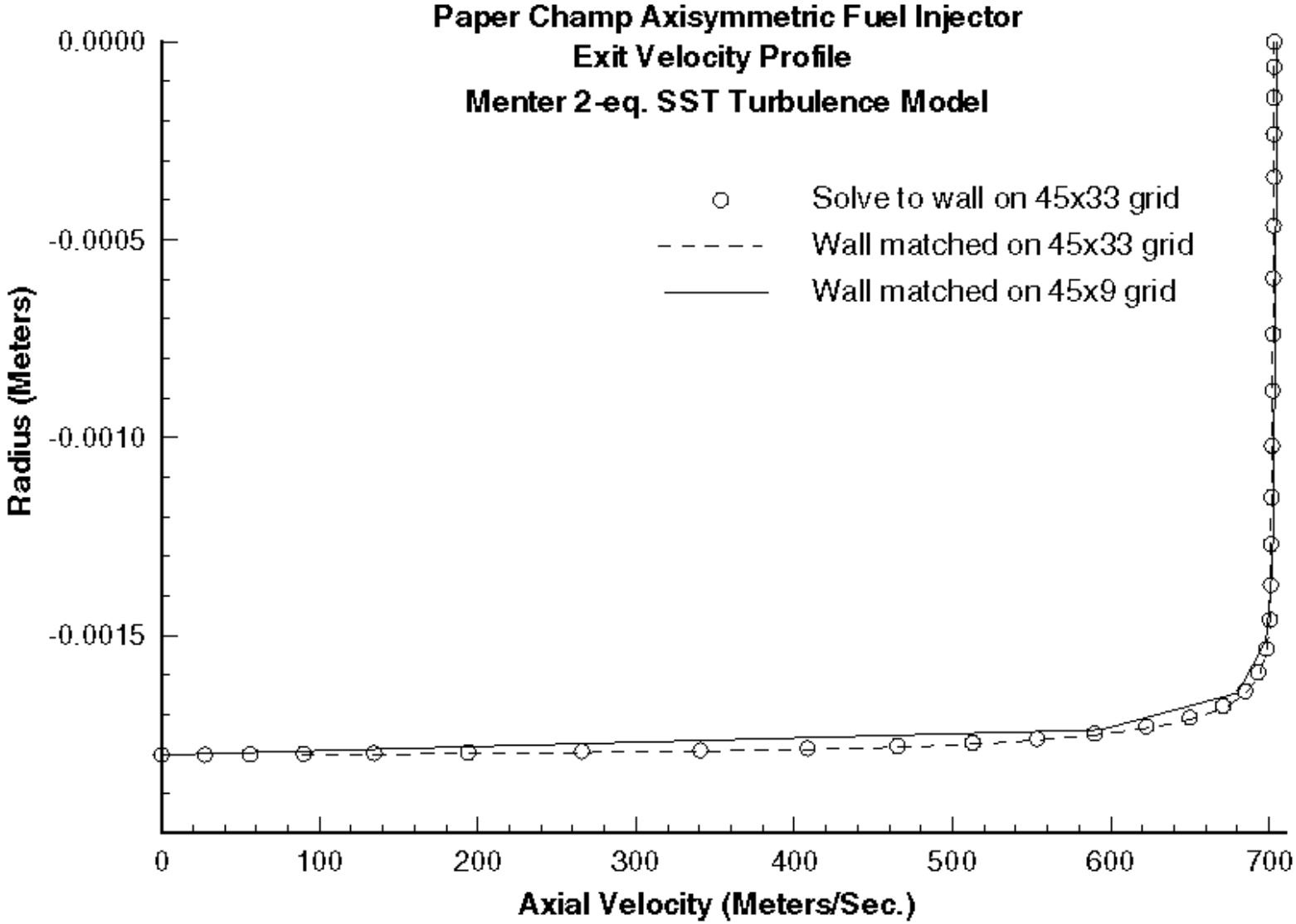
Objective: Simulation of fuel injector flow as well as passage flow.



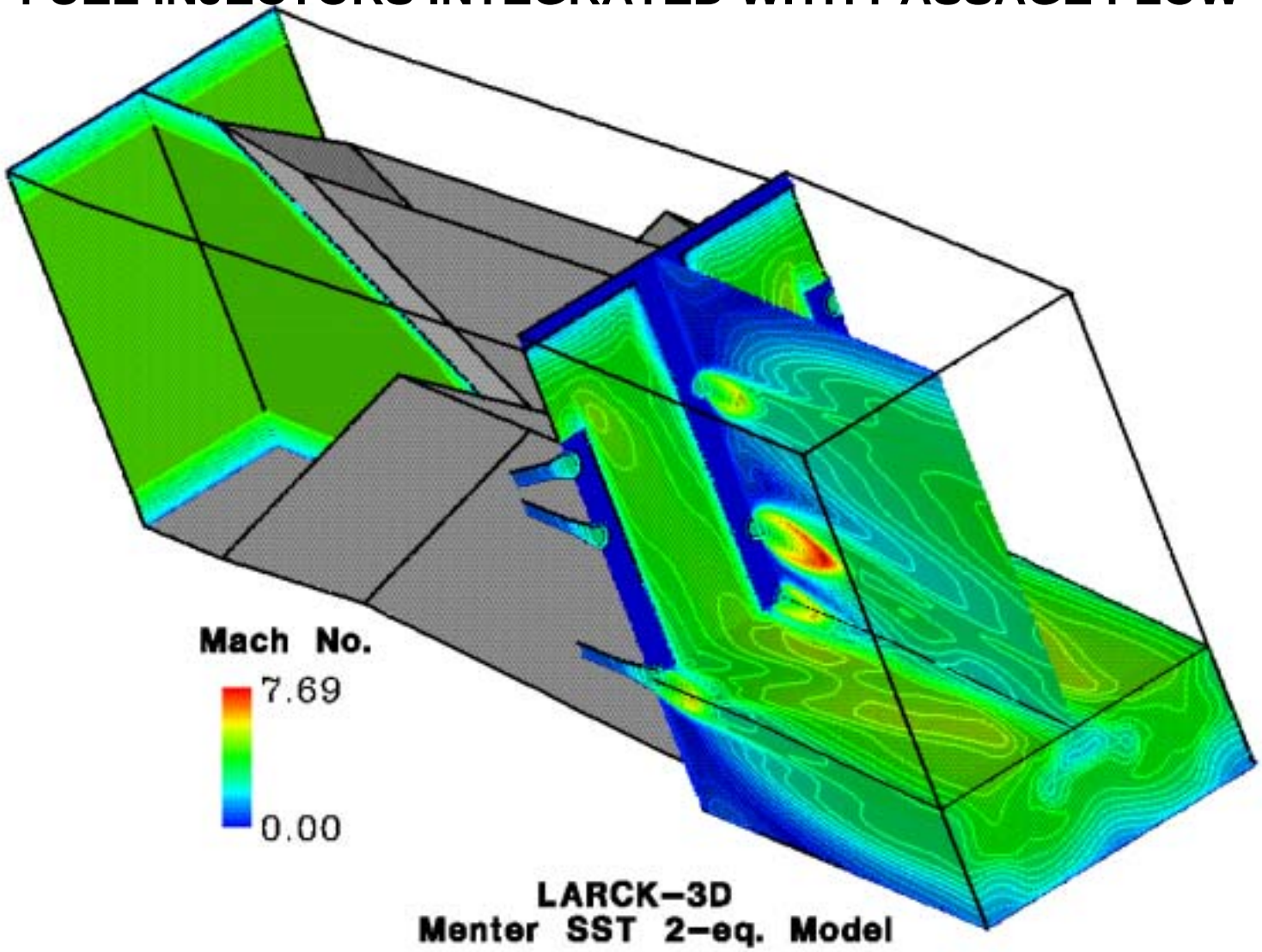
PAPER CHAMP FUEL INJECTOR SIMULATION STUDY : A COMPARISON OF 3-D AND AXISYMMETRIC MODELS



PAPER CHAMP FUEL INJECTOR SIMULATION STUDY : A COMPARISON OF WALL TREATMENT AND GRID RESOLUTION



PAPER CHAMP FUEL INJECTOR SIMULATION STUDY : FUEL INJECTORS INTEGRATED WITH PASSAGE FLOW



CHEMISTRY TURBULENCE MODELS

Turbulence interactions with the chemical kinetics are modeled using either mixed is burned or variance+PDF models :

- Mixed is burned model based on the eddy dissipation concept of Magnussen et. al. **(NEW)**

- Chemistry turbulence models (turbulent species production/destruction) are currently modeled as de-correlated.
  - Energy variance + a scalar assumed Beta Probability Density Function (PDF) for the effect of temperature fluctuations on the reaction rate coefficients ($\mathbf{k}_f$ and $\mathbf{k}_b$)
  - Sum of species variance + multivariate assumed Beta PDF for the effect of the species fluctuations on the species production/destruction.

- A new two equation turbulent scalar diffusion model for species diffusion is currently under development through a NGLT grant. **(NEW)**

TIME/SPACE INTEGRATION ALGORITHMS

- Spatially and temporally explicit schemes:
  - Second order time accurate Runge-Kutta scheme (global time step).
  - Steady state Runge-Kutta scheme (local time step) with or without residual smoothing.

- Spatially and temporally implicit schemes:
  - Steady state diagonalized approximate factorization (local time step DAF).
  - Steady state block approximate factorization (local time step BAF).
  - Steady state diagonally dominant alternating direction implicit (local time step DDADI).
  - Second order time accurate implicit dual time-stepping scheme using 2^{nd} order backward temporal differences. **(NEW)**
  - Second order time accurate implicit dual time-stepping scheme using Crank-Nicoloson method. **(NEW)**

CONVERGENCE ACCELERATION

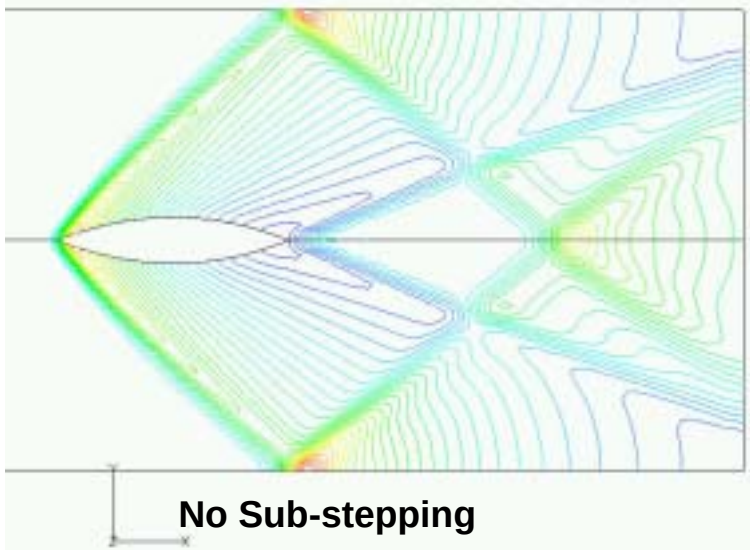
- Convergence acceleration can be accomplished using either:
  - Full coarsened coarse-to-fine grid sequencing:
    - Solve on a coarsened grid with a robust scheme (e.g. a 1st order scheme).
    - Interpolate from the coarsened grid to the next finer grid level and then solve.
    - Repeat until fine grid is reached and then switch to a higher order scheme.
  - Full coarsened V or W-cycle full approximate storage multi-grid (FAS).
  - Full coarsened full multi-grid (FMG : A combination of coarse-to-fine grid sequencing and V or W FAS)

- Coarse-to-fine sequencing works well for wide variety of flows.
- Multi-grid a good approach for elliptic flows only when computational grid is very fine.

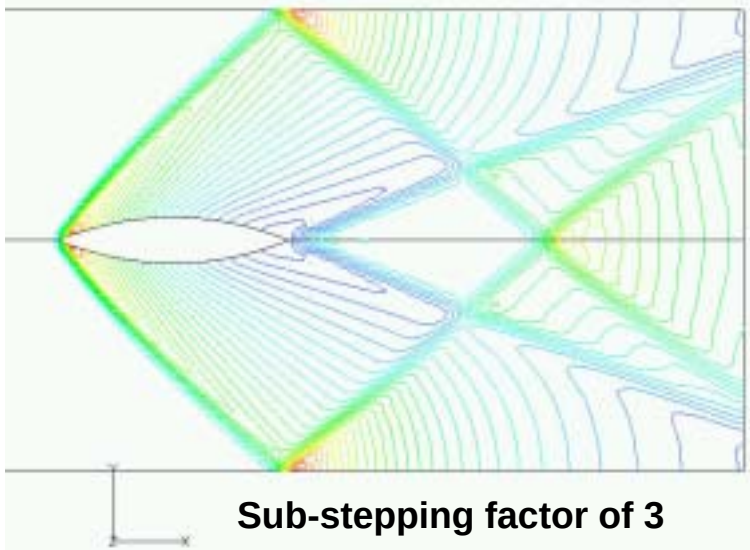
- Coarse-to-fine sequencing and multi-grid have been found to work very well with space marching scheme.

SUB-STEPPING FOR SPACE MARCHING

- Allows the user to linearly refine the grid in the marching direction without regenerating the grid.
- Can be used to help remove numerical oscillations in the space marching direction by either:
  - Reducing the size of the gradient used in the second order fully upwind flux construction.
  - Allow the user to switch to a 1st order fully upwind streamwise flux construction.



No Sub-stepping



Sub-stepping factor of 3

PHYSICAL AND INTRA-BLOCK CONDITIONS

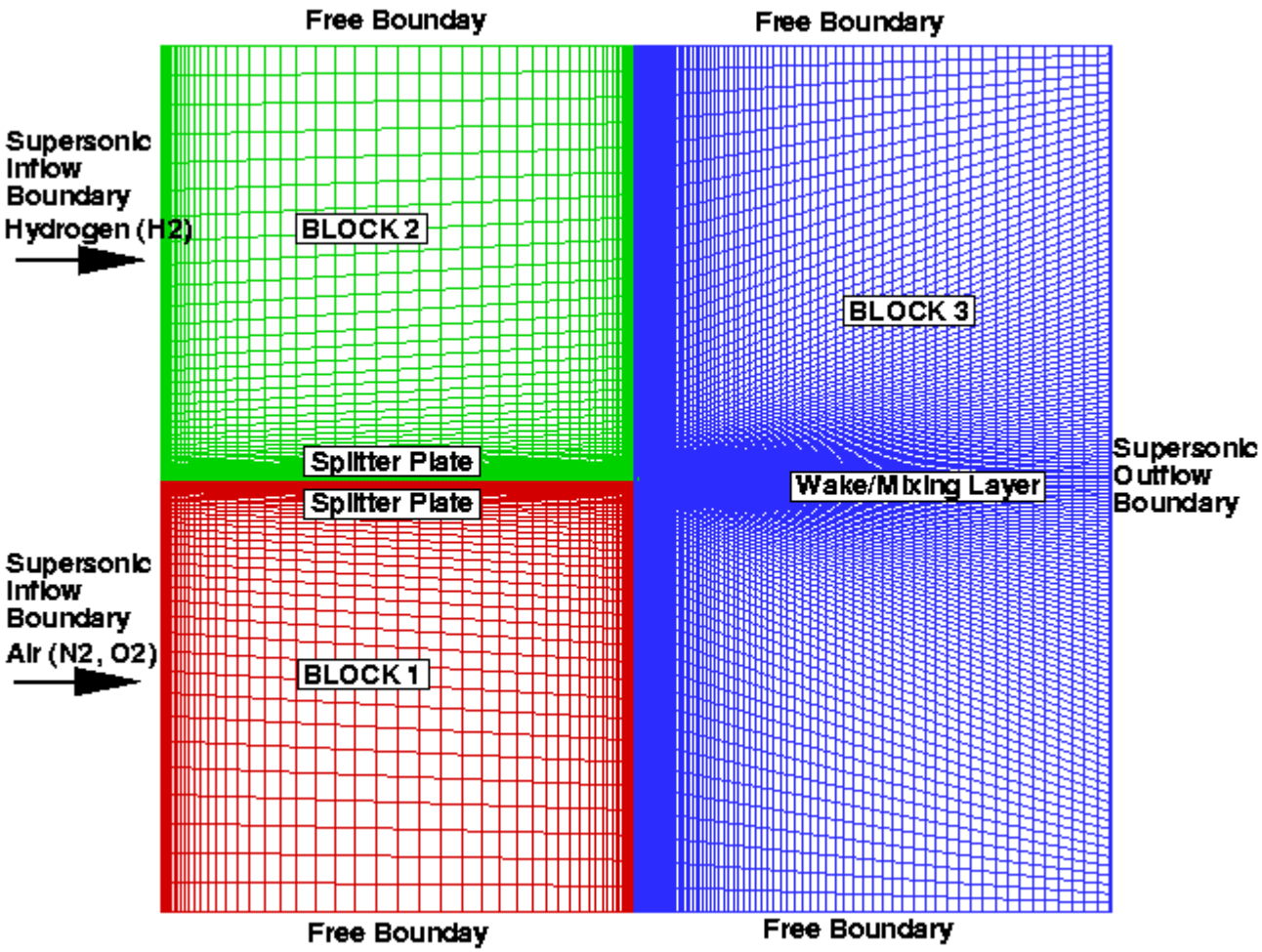
- There are seventeen different types of boundary conditions implemented which:
  - Can be specified on any boundary or subset of a boundary.
  - Can be treated explicitly or implicitly (depending on time/space integration scheme used).

- There are two types of intra-block (block-to-block) boundary conditions:
  - CUTS : C(0) (point wise continuous) block-to-block connectivity that:
    - Can be specified on any boundary or subset of a boundary.
    - Are fully second order accurate when grid is smooth.
    - Are fully conservation preserving when flux telescopes.
  - PATCHES : Non-C(0) (point wise discontinuous) block-to-block connectivity that:
    - Can be specified on any boundary or subset of a boundary.
    - Are fully second order accurate when grid is smooth.
    - Are weakly conservative.

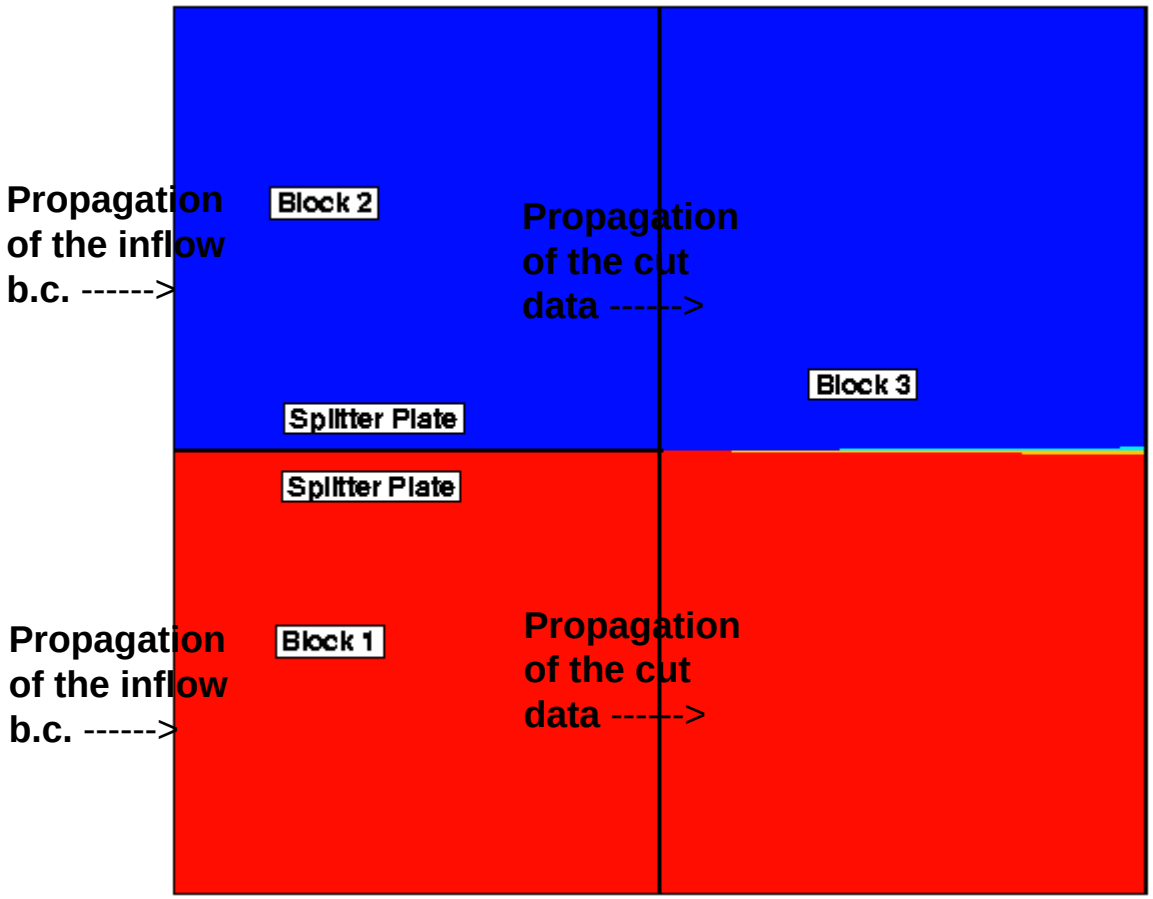
FLOW INITIALIZATION

- Experience has shown that as applications become more complex the initial guess plays an increasingly important role.
- There are seven different types of flow initialization methods implemented to provide flexibility in specifying the initial guess.
  1) The reference conditions are always used to set a default initialization of all cells in all blocks and regions.
  2) Initialization by propagation of physical boundary condition ghost cell data.
  3) Initialization by propagation of 'INITIAL' boundary condition ghost cell data (these b.c. are ignored during solution process).
  4) Initialization by a 'BLEND'ed propagation of any boundary condition ghost cell data.
  5) Initialization by propagation of CUT ghost cell data.
  6) Initialization by propagation of PATCH ghost cell data.
  7) C-D nozzle one-dimensional initialization.

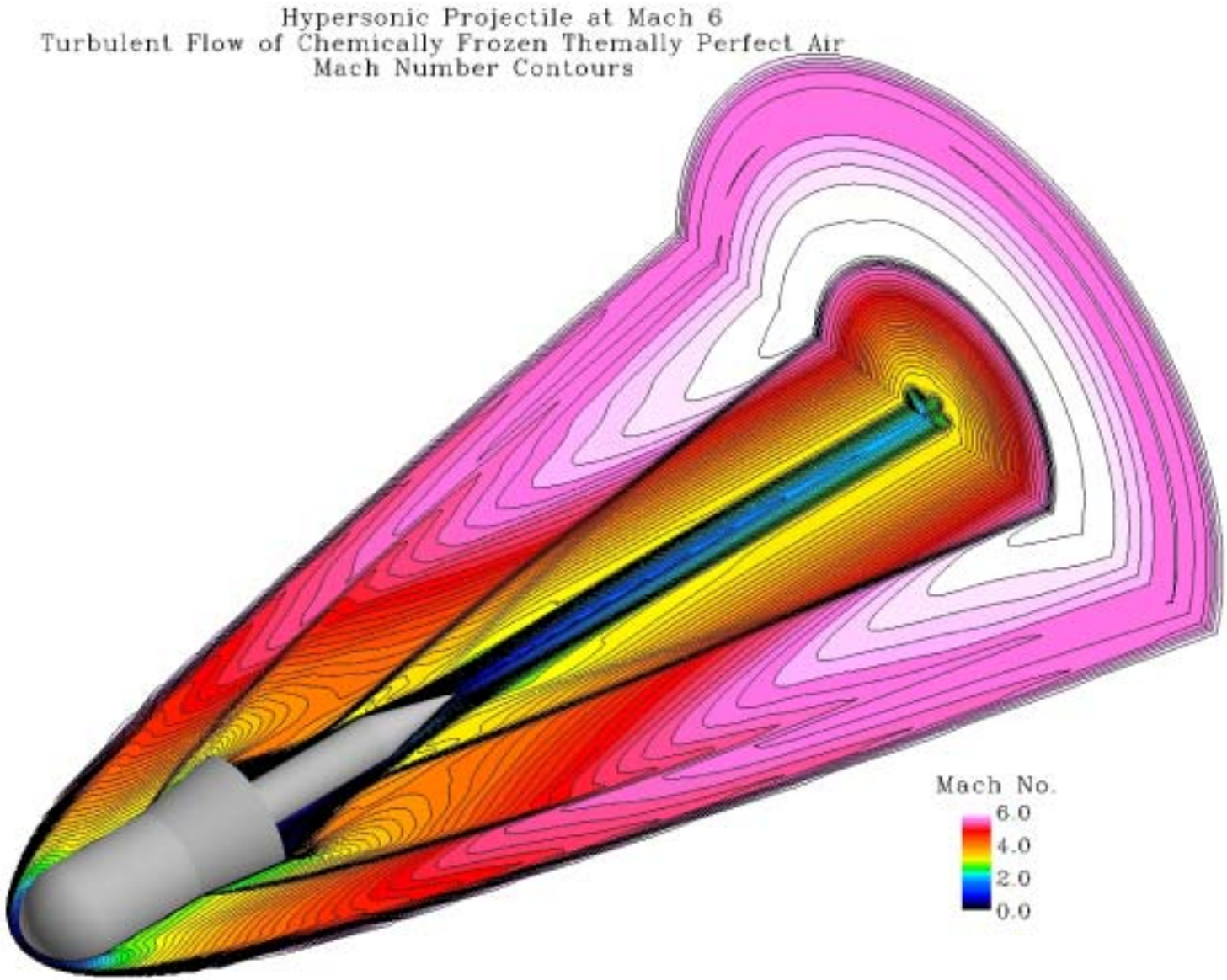
FLOW INITIALIZATION EXAMPLE (PROPAGATE)



FLOW INITIALIZATION EXAMPLE (PROPAGATE)

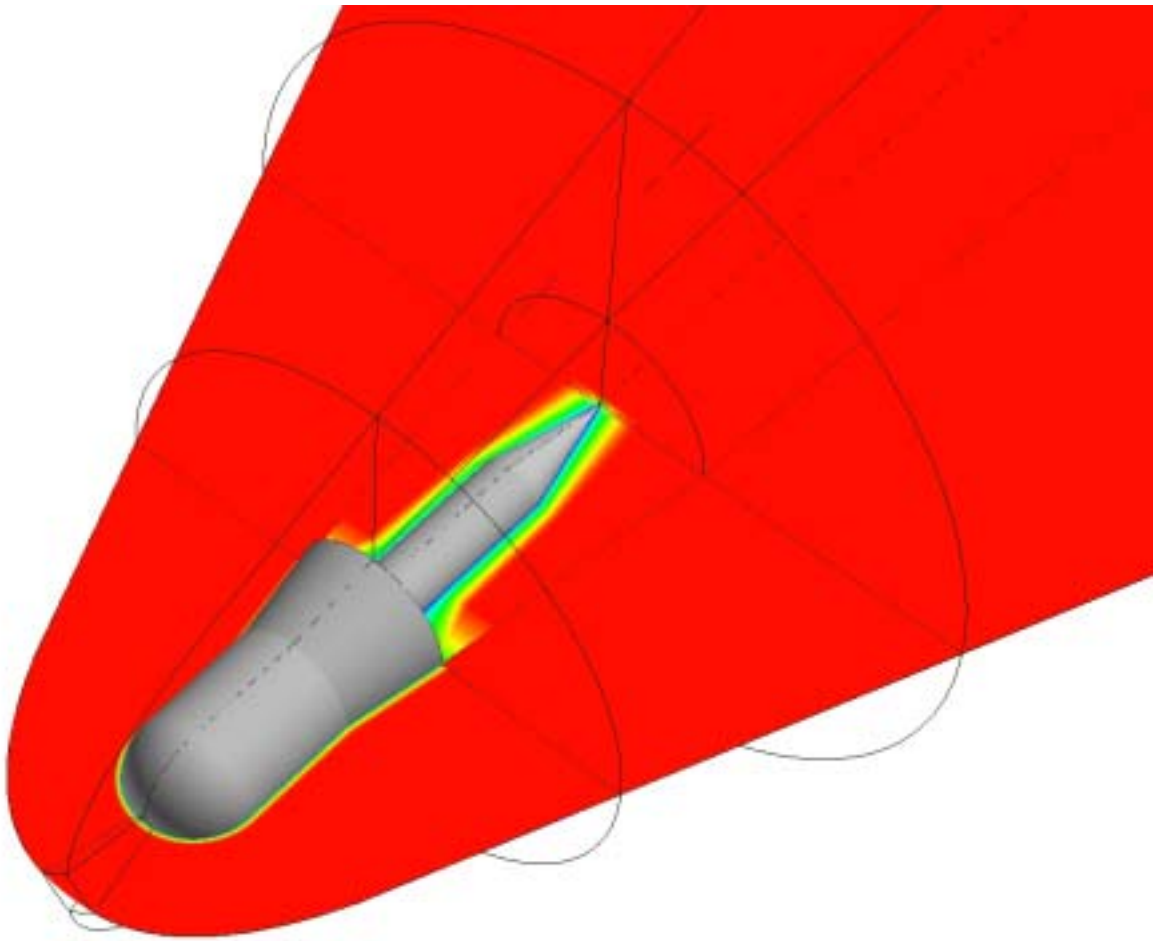


FLOW INITIALIZATION EXAMPLE (BLENDing)



FLOW INITIALIZATION EXAMPLE (BLENDing)

Mach 6 Projectile



LAMINAR AND IGNITION SUB-BLOCKS

- Laminar sub-block are a group of cells within a block for which the turbulent source terms are turned off.

- This is done in such a manner that the code:
  - Passively advects the inflow turbulence b.c.'s. and resets the turbulence eq. wall b.c.'s in the sub-block.
  - Provides a way to control where flow becomes turbulent.

- Ignition sub-blocks are a group of cells within a block where a minimum user specified static temperature is enforced.

- This is done in such a manner that the code:
  - Adds energy to the flow in the sub-block.
  - Provides a way to "spark the flow" or force ignition when and where needed.

CODE INTERFACES AND POST-PROCESSING

- The VULCAN input file generation graphical user interface can read and extract two kinds of information from the Gridgen generic flow solver file.
    - Physical b.c.'s.
    - Intra-block C(0) connectivity data.
- The VULCAN post-processor writes I-blanked plot3d grid, and either Q or function files and a Fieldview name file.
- The VULCAN post-processor can be made to write out the conserved variables contained in the cells adjacent to a physical b.c. into a "profile file".
    - Profile files can be read by VULCAN and treated as b.c.'s
    - Profile files can be used to provide data to external codes
- The VULCAN post-processor automatically integrates the forces, moments and heat loads of all "walls" and flow-thru b.c.'s in the computational domain and summarizes them by :
    - Each individual b.c. type (wall or flow-thru)
    - The sum of the each b.c. type in each block.
    - The sum of all b.c. types in the computational domain.
- The VULCAN post-processor automatically writes a file containing the y+ of the 1st cell center off-the wall, the wall PdA components, shear force components, heat flux and cell face area of all wall b.c.'s to a file.

CODE GRAPHICAL USER INTERFACE (GUI)

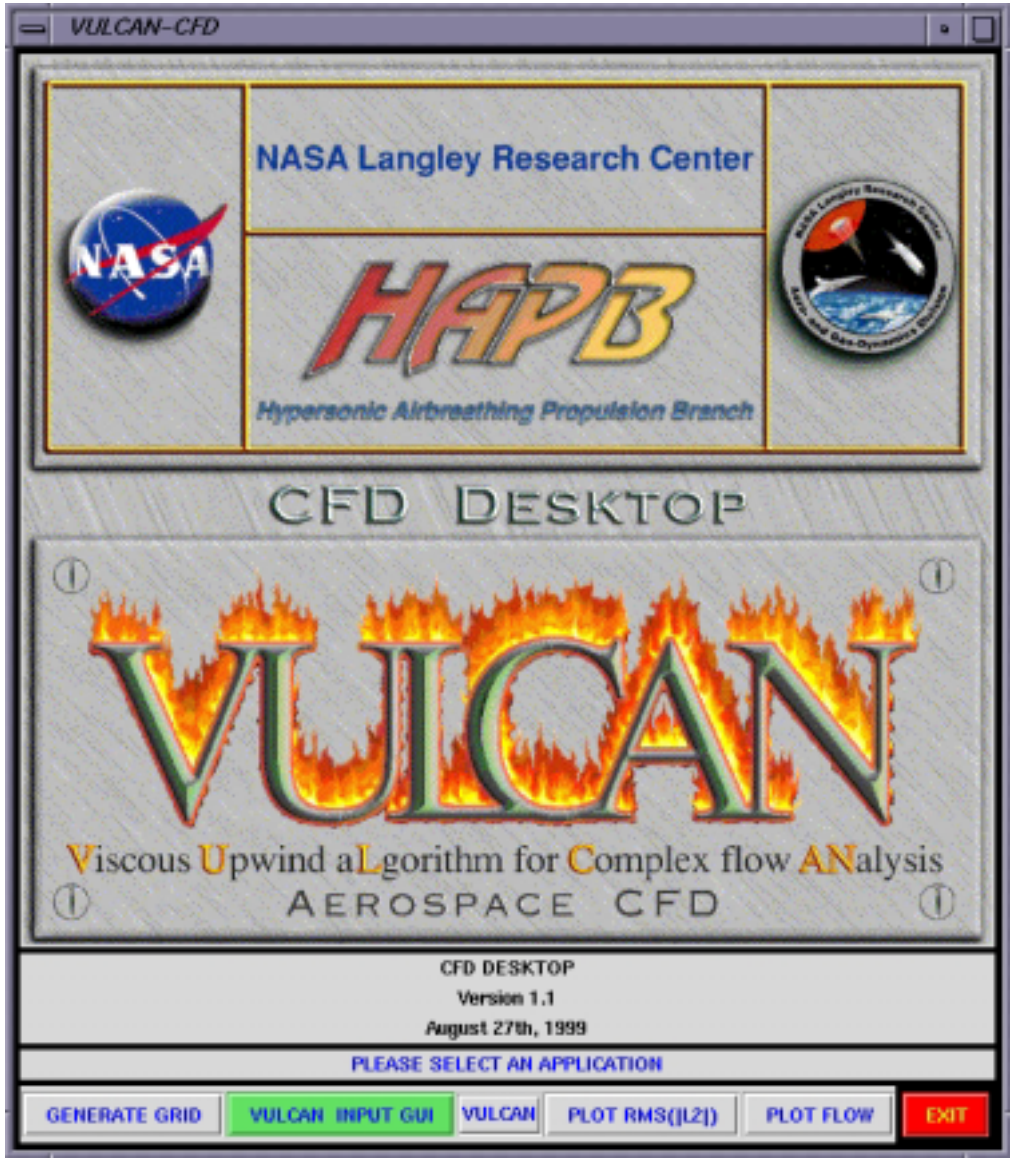
Two **tcl/tk** based GUIs are supplied with VULCAN

• **VULCAN-CFD** : A desktop GUI to provide an API that connects the CFD process tools together,
  • Grid generation tool (Gridgen, ICEM, Tecplot, …)
  • VULCAN input file GUI
  • VULCAN
  • Residual history plotting tool (Tecplot, …)
  • Graphical Post-processor tool (FIELDVIEW, Tecplot, ICEM, …)

• **VULCANIG** : An input file GUI/wizard to provide a quick way to create VULCAN input files with error checking and interfaces to Industrial grid generation codes for the importation of block connectivity and b.c. information.
  • Gridgen generic flow solver file importation.
  • ICEM VULCAN input file importation.

Overview

VULCAN-CFD



VULCANIG