

Appendix A

Technical specification of Star CCM+ CFD tool

S NO.	SPECIFICATION	DETAILS
1.	License type	Star CCM+ CFD tool, Power session, Perpetual Licence with at least one-year free updates. With additional 10 DOE tokens
2.	General requirement	Computational fluid dynamics (CFD) software for solving multidisciplinary problems in both fluid and solid continuum mechanics, within a single integrated user interface (GUI). The analysis software should enable CFD workflow process using a single file for solving problems involving compressible, incompressible flow (of fluids), heat transfer, multiphase, particulate flow (based on Lagrangian and Discrete Element Method descriptions), theology, electromagnetic, extreme motion, and solid stress. The software's environment should offer all stages of engineering analysis within a single graphical user interface which should include: 1. Import and creation of geometries that are simple and complex in their topologies. 2. Edit imported geometries using either solid body operation or surface modelling. 3. Ability to generate structured and unstructured meshes with different cell types and topologies. 4. The solution of the governing equations for a specific class of problem on UNLIMITED HPC cores with a single license. 5. Analysis of the simulation results. 6. Automation of the simulation workflows using different techniques not limited to scripting. 7. Connection to other CAE software for co-simulation analysis.
3.	Application feasibility	Key applications and capabilities that should be addressed by the CFD software are as follows: 1- Surface cleanup of complicated geometry. 2- Perform and evaluate aerodynamics studies. 3- Optimize body shape to minimize/maximize intended performance metrics (such as drag, lift, etc.). 4- Internal flow through nozzle – plume interaction 5- External, Internal flow at High Mach No. 6- Motion modelling for separation studies 7- Heat Flux, Real gas for re-entry vehicle at different altitude 8- Combustion 9- Cavitations modelling under water 10-Incompressible flow in air, water 11-Post processing the results [Scalars, Vectors, XY plots]



Detailed technical specification	
S No.	Specification
1	Geometry modelling A fully featured in-built CAD modeller within the software's GUI enabling geometry modelling and manipulation with the following features: <u>Geometry Import-</u> • License-free import of Neutral formats - IGES, STEP, Parasolid, IDF, and NX part files • Import Triangulated formats - STL, pro-STAR .dbs/.inp, NASTRAN and PATRAN shells .nas and .pat • Import of PLM formats such as PLMXML • Invoke automatic error checking and healing upon CAD import • Import interoperable volume mesh formats such as Fluent case file (*.cas, .grd, .msh), plot3d mesh file (*.grd, .msh, .p3d, .xyz, .x), cgns mesh file (*.cgns, .cga, .cgh) <u>Geometry Creation and Modification features—</u> • A fully parametric feature-based modeller is built upon the Para solid kernel. Works both on Linux and Windows OS and can be fully integrated within the client-server architecture of the software.
2a	Surface Repair Surface meshing tools should provide high-quality triangulations on arbitrarily complex and dirty geometries. The following surface meshing tools should be provided 1- Surface preparation: to manually repair and prepare surfaces ready for meshing (quads and triangles) 2- Surface wrapper: Provide a closed, manifold, non-intersecting surface when starting from quality CAD data 3- Surface mesher: to provide a high-quality starting surface for all volume mesh types 4- 2D Mesher - to create triangular and polygonal meshes on 2D Geometries. 5- Surface wrapper: A surface wrapper is a crucial tool for preparing quality CAD data for simulation purposes. It ensures that the geometry is closed, manifold, and non-intersecting, making it suitable for mesh generation in CFD, FEA, and other simulation types. By automating the repair of geometry issues, surface wrappers ensure that simulations are run with accurate, reliable models, saving time and reducing errors in complex simulation setups.
2b	Meshing A fully inbuilt structured and unstructured masher should be available to discretize simple and complex shapes <u>Mesh topologies to support:</u> 1. Surface - Triangles, Enhanced triangle, Quadrilaterals, and Polygons 2. Volume - Tetrahedron, Hexahedra, Prims, arbitrary Polyhedral The meshing framework should provide a flexible environment to execute meshing operations in a repeated manner without any user intervention. It should be possible to execute the following features: 1- Sequence and re-order mesh operations 2- Serial, Con-current per part, and parallel mesh generation techniques is available



- 3- Local mesh modification of wrapped and remeshed surfaces
- 4- Automatic Conformal polyhedral and tetrahedral meshes across interfaces and multi-part/region assemblies

The software should provide automatic volume mesh generation with optimized cell quality for arbitrarily complex geometries. Volume meshers should include core general meshers as well as meshers designed for specific features such as long pipes and/or thin regions.

Core Mesher models are to be made available-

- 1- Trimmed cell mesher with anisotropic size support
- 2- Polyhedral mesher
- 3- Tetrahedral mesher
- 4- Prism layer mesher
- 5- Advancing layer Mesher

Specialized Meshers required-

- 1- Thin mesher
- 2- Generalized cylinder mesher
- 3- Extruder mesher
- 4- Offset mesher

Directed mesher for swept geometries-

- 1- Manual or automatic creation of patches for sweeping
- 2- Control of layer count/cell size and distribution
- 3- Rotational sweep coarsening for sector meshes

Trimmed cell mesher

A **trimmed cell mesher** is a powerful and efficient tool used to generate high-quality meshes for complex geometries. By adapting the mesh to the shape of the object, it ensures that simulations are accurate, computationally efficient, and reliable. Whether in CFD, FEA, or multiphysics simulations, the trimmed cell mesher provides a means of handling intricate shapes and complex boundaries, ensuring that the computational domain is accurately represented for the most precise simulation results

3 Solver

The software should contain numerical algorithms that solve systems of equations constructed from the chosen physics models and supplied boundary conditions.

Details of the solver are as below-

- 1- Choice of Mixed or Double-precision implementation
- 2- The solver is to be based on the Finite Volume method based on the Algebraic multigrain linear method with the following features-
 - a. *Segregated flow* solver with automatic continuity initialization
 - b. *Coupled flow* solver with solution acceleration techniques like Automatic CFL control and explicit under-relaxation, Grid Sequencing Initialisation (GSI), and Continuity Convergence Acceleration (CCA)
 - c. *SIMPLE* and *PISO* solution algorithms
 - d. Choice of using Harmonic balance method for periodic unsteady flows and single frequency electromagnetic where applicable
 - e. Option to choose, for convection,
 - the 1st Order upwind, 2nd Order upwind, central-differencing (Regular and bounded), Hybrid second-order upwind/CD (regular and bounded), hybrid MUSCL 3rd-order/CD
 - f. Option to choose for time, first-order (Euler implicit) and



	second-order discretization 3- The software should enable users to choose the finite element solver based on the application with the following features- - Shared or distributed memory linear direct solvers - In-core or out-of-core memory storage - Memory estimation before running - Multi-threading capability - Applicable to simulate problems involving Solid stress, Viscous flow, and Magnetic Vector Potential 4- The Finite element solver should be compatible with Parallel Execution including automatic decomposition, parallel disk I/O and have compatibility with different MPI technologies namely Open MPI, Microsoft MPI, SGI MPI, and Cray MPI
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4 Applications

a) General fluid dynamics

The software should be able to handle problems that are multi physical in nature. Users should be able to setup the physics to be simulated using different physics models that are based on fundamental laws of physics. Users should be able to simulate scenarios with multiple time scales combination (Steady-Unsteady, Steady only, Unsteady only) within the same simulation file for different regions of discretized domain.

Physics capabilities should cover the following –

Flow Characteristics:

- 1- Inviscid, laminar, or turbulent
- 2- Newtonian and Non-Newtonian viscosities
- 3- Incompressible and compressible
- 4- Multi-component mixtures
- 5- Multiphase
- 6- Porous resistance
- 7- Gravitational acceleration
- 8- Passive scalars

Temporal discretization:

- 1- Steady
- 2- Unsteady (explicit, Implicit, and PISO)

Equation of State:

- 1- Constant density
- 2- Ideal gas law
- 3- Real gas law (Peng-Robinson, Redlich-Kwong, Standard and Modified Soave-Redlich-Kwong, Van der Waals, Equilibrium Air, IAPWS-IF97)
- 4- Polynomial density
- 5- User-defined equation of State

Heat transfer-

The software should be able to simulate different modes of heat transfer (Conduction, Convection, and Radiation) in both fluid and solid materials. Radiation (Surface to Surface (S2S)) with view factors for both gray and multiband, Surface photon Monte Carlo, solar loads, discrete ordinate model (DOM) or P1 for participating media)

Turbulence-

The software provides an out of box choice of turbulence models for



modelling different flow behaviours-

Reynolds-Averaged Navier Stokes (RANS) –

- 1- Spalart - Allmaras (standard and high-Reynolds number)
- 2- K-Epsilon (standard, realizable, two-layer, low-Reynolds number, elliptic blending, lag elliptic blending, and V2F)
- 3- K-Omega (standard and SST)

Reynolds Stress Transport models with :

1. Linear pressure strain (standard and two-layer)
2. Quadratic pressure strain
3. Elliptic blending

Large Eddy Simulation (LES)-

1. Sub grid scale models (Smagorinsky, dynamic Smagorinsky, and WALE)

Detached Eddy Simulation (with delayed and improved delayed)

SST K-Omega with-

1. Spalart-Allmaras
2. Elliptic blending

Initial and Boundary Conditions for LES and DES

1. Synthetic turbulence
2. Anisotropic Linear Forcing (ALF)

Transition and suppression modeling -

1. User-defined turbulence suppression
2. Gamma ReTheta model
3. Gamma model

Miscellaneous associated Models

1. Temperature heat flux model

Wall treatments (high-y+, low-y+, and all-y+)

b) Physics-based mesh adaption

The software should provide *solution-based dynamic refinement* and coarsen of mesh for both polyhedral and trimmed hexahedral mesh with the following features-

1. User-defined and model-driven adaption criteria
2. Inbuilt Model-driven adaption for multiphase VoF, Overset meshes, and reacting flow
Automatic re-partitioning and balancing upon adaption for parallel scalability

c) Motion Dynamics

The software can model moving entities, deforming meshes, and multiple frames of references with the following options for its specification-

1. User-defined *rigid body motion* (Rotation, Translation, and trajectory)
2. **Dynamic fluid body interaction (DFBI) –6DOF**
 - a. The model motion of bodies in six degrees of freedom under the action of fluid forces-
 - i. Ability to represent bodies both as a continuum or mechanical (meshless) type.
 - b. Ability to incorporate Superimposed motion
 - c. Specification of *Body-body couplings* and external forces
 - d. *Contact prevention models* is supported



d) Reacting flows

The software should be able to simulate chemical processes that occur in combustion, polymerization, and other chemical reactions with the following features:

Fuel types supported- Solid, Liquid & Gas with

Premixed, partially premixed, and non-premixed combustion models

Out of the box models for simulating-

1. General gas-phase chemistry
2. Liquid-liquid chemistry
3. Interphase reactions
4. Surface reactions
5. Particle reactions and coal combustion
6. Polymerization

Combustion models available out of the box-

Flamelet-

1. Flamelet Generated Manifold model (FGM)
2. Steady Laminar Flamelet (SLF)
3. Chemical Equilibrium
4. Flame propagation models
 - a. Coherent Flame Model (CFM)
 - b. Turbulent Flame Speed Closure model (TFC)
 - c. Thickened Flame Model

Reacting Species Transport –

1. Complex Chemistry:
 - a. Laminar Flame Concept
 - b. Eddy Dissipation Concept
 - c. Thickened Flame Model
 - d. Turbulent Flame Speed Closure model (TFC)
 - e. Relaxation to Chemical Equilibrium
2. Eddy Break-Up model (EBU):
 - a. Standard or Hybrid EBU
 - b. Combined Time Scale
 - c. Kinetics Only
 - d. Thickened Flame Model
3. Eddy Contact Micro mixing (ECM)
4. Additional models:
 - a. NOx emissions
 - b. Soot emissions
 - c. 1D reacting channel
 - d. Spark Ignition
 - e. Combustor Reactor Networks

e) Multiphase flow

The software should be capable of handling multiphase flow both in Eulerian and Lagrangian descriptions capturing distinct fluid phases within a single simulation.

Eulerian Multiphase (EMP) Segregated Flow with-

1. Support phase types of gas, liquid, and particle (granular)
2. Support interphase energy, momentum, and mass transfer and have



- relevant models available to model these phenomena out of the box
3. A Large scale interface model (LSI) to capture hybrid nature of mixed regime flows
 4. Granular phase models based on granular pressure, and granular temperature transport (Energy)
 5. Population balance models for disperse phase prediction using S-Gamma and A-MUSIG
 6. Crystallization using Single component crystal growth
 7. Wall and bulk boiling models
 8. Phase-wise turbulence modeling and chemical reactions

The Volume of Fluid (VOF) -

1. Ability to solve the conservation equations for the volume fraction of one distinct phase
 - a. Single and multi-step implementation is supported
2. Track the *free surface* between immiscible fluids using a *High-resolution interface capturing (HRIC)* scheme
3. Ability to model Phase-change processes: *evaporation and condensation, boiling, cavitation, gas dissolution, melting and solidification*
4. Direct connection to adaptive mesh refinement technology
5. Models *Cavitation*
 - a. *Full Rayleigh–Plesset* (for single-component phases) or *Multi-component Full Rayleigh–Plesset* (for multi-component phases)
 - b. *Schnerr-Sauer* (for single-component phases) or *Multi-component Schnerr-Sauer* (for multi-component phases)
 - c. *Homogeneous Relaxation* (for single-component phases) or *Multi-component Homogeneous Relaxation* (for multi-component phases)

Fluid Film-

1. Ability to predict film formation through user initialization, injection through a boundary, or impingement from other phases
2. Compatibility with Edge or wave stripping
3. Ability to model Phase-change processes: evaporation and condensation, boiling, melting, and solidification
4. Option for Mass removal from the frozen film in conjunction with mesh morphing to simulate ice accretion

Dispersed multiphase (DMP) -

1. Option to choose an approach that solves for the dispersed phase in a Eulerian manner with one-way or two-way coupling
2. Compatible with the formation of fluid films

Mixture Multiphase (MMP)

1. The software should provide a simplified multiphase model for modelling mixture flows

Lagrangian Multiphase (LMP)-

The software should handle the particulate type of flow processes such as that involving the transport of solid particles, liquid droplets, or gas bubbles—known as dispersed phases—by gaseous or liquid continuous phases. Additionally, the following features are required-

1. Ability to account for Particle equation of motion: drag, pressure gradient, virtual mass, gravity, and body forces
2. Compatible with multi-component liquid and solid particles



descriptions

3. Ability to model Heat and mass transfer
4. Option to simulate Impingement erosion
5. Inbuilt Atomization and breakup models for particles is available
6. Ability to account for and simulate Collision and coalescence
7. Compatible with Passive scalar interactions
8. Option to Mass transfer into VOF phases
9. Ability to model particle interaction with Coulomb forces
10. One/Two-way coupling model with underlying continuous phase along with cell clustering technique enabling user-defined settings for source smoothing is provided

The software has the in-built capability for simulating flows involving Discrete Element Method (DEM) with the following features-

1. Ability to simulate large numbers of interacting discrete objects
2. Model the Particle equation of motion—resolve rotation of particles
3. Inbuilt Models for particle-particle contact and particle-boundary interaction
4. Models for Particle bonding and breakup
5. Availability of Spheres, cylinders, capsules, polyhedral, composite, clumped, or coarse grain type of particle shapes
6. Models to handle Particle-particle, particle-boundary, and particle-continuous phase heat transfer.
7. Ability to simulate Erosion of walls due to particles: abrasive and impact wear
8. One/Two-way coupling model with underlying continuous phase along with cell clustering technique enabling user-defined settings for source smoothing is provided
 - a. There is an option to couple phases once per time step and within the inner iteration of fluid time step if required.

For *Particle injection*, the following Injectors entities are available -

1. The point, part, and surface
2. Tabular
3. Size distribution functions
4. Hollow and solid cones
5. Pressure swirl
6. Lattice
7. Random region input

f) Solid Mechanics

The CFD software should provide an integrated finite element solver for the solution of solid mechanics, fluid-structure interaction, heat conduction, electromagnetics, and thermal stress problems with the following features:

1. Static dynamics and quasi-static analysis
2. Option to select linear and non-linear geometry with full and modified Newton matrix update
3. Support for 3D linear and quadratic solid elements - Hexahedra, tetrahedral, wedge, and pyramid types
4. Ability to model Isotropic, Orthotropic, and anisotropic linear elastic materials; Hyper elastic and elastoplastic materials
5. Availability of Rayleigh damping
6. Loads and constraints for points and surfaces; body loads
7. Thermal stresses from mapped or computed temperature fields
8. Cyclic symmetry boundary conditions



	9. Bonded and small sliding frictionless contacts for conformal and non-conformal meshes 10. One way and two-way Fluid-structure Interaction (FSI) with added mass pre-conditioner Ability to model contact employing frictionless contact with infinity rigid plane
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5	Post Processing/ Data analysis The software should have comprehensive post-processing capability fully inbuilt into the same GUI. The post-processing capabilities enable live and in-situ monitoring of results while a simulation is running. 1- Provides a computed summary of engineering quantities for example force, system parameters for example memory usage, simulation metrics for example solver elapsed time, any user-defined functions, statistical functions for example the mean, mathematical functions for example integrals. 2- Provide a basis for facilitating sampling and saving of information in a summarized manner from the simulation during the solving process. 3- The software should facilitate the creation of two-dimensional plots of different types namely, the time history of a sampled quantity, imported tabular data, histograms bar charts, 3-way bubble plots to visualize data while the size and colour scaling with another function simultaneously. 4- The software should have comprehensive techniques to visualize the simulation results in form of scalar and vectors using varied data sets such as surface, volume, and discredited entities. a. Visualize the following post-processing entities i. Scalar field display ii. 2D and 3D Vector glyphs iii. Pre-defined colorcast with tools for creating new ones iv. Streamlines v. Volume rendering of scalar fields vi. Line Integral Convolution for vector fields vii. Section slices viii. Iso-surfaces ix. Display of DFBI bodies, forces, and couplings x. The point, line, grid, and arbitrary probes xi. Scalar and Vector wraps for showing exaggerated deformations 5- Ability to generate user-customizable HTML reports that details the settings for a specific simulation file. 6- Facility to record snapshots of simulation data at different instances on various simulation entities such as surfaces, volume, derived entities, and Particles onto a history file. 7- Provision to interrogate simulation data on the XY plot connected to a 3D Scene using heat map-canvas selection filters. 8- Fully inbuilt and integrated animation tool based on key frame animation technique allowing to setup time-based control for a wide range of visualization properties. 9- A license-free external virtual reality (VR) client developed by the vendor directly is provided having the following features: a. Provide standalone and ability to connect to a running simulation to provide in-situ results visualization using VR techniques.
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	b. Model manipulation using handheld controllers namely pan, zoom, and fly. c. Ability to provide mass less particle emitters to track the flow field. d. Ability to allow multiple VR connections to visualize the VR scene.
6	Design Exploration
	A fully inbuilt add-in that enables automated approach for running design exploration studies covering performance studies.
7	Connection to external CAE software
	Software should provide internal coupling to the following tools – 1- System/ 1D tools - GT Suite, Simcenter AMESIM, RELAPS-3D, and WAVE 2- 3D simulations tools - Simcenter STAR-CCM+ (Cosimulation mode only), Abaqus and Simcenter NASTRAN The software should provide its internal co-simulation API to allow third part/user-specific tools to create coupling interfaces. Co-simulation through Functional mockup interface (FMI) is supported out of the box to run co-simulation with FMU compliant with standard 1.0 and 2.0. File-based coupling between the software should be provided out of the box with traditional CAE file such as from- 1- Abaqus, using .inp files 2- Ansys, using .cdb files 3- Nastran, using .nas, .bdf or .dat files 4- TAItherm, using .ntl or .neu files 5- RCAS, using .in files 6- Import and Export of CGNS files. There is a provision to visualize the import CGNS data along with geometry definition and engineering field (Scalar and vector) input. Data mapping techniques should be available out of the box to interpolate data to or from different meshes and entities. 1- Surface to Surface, volume or beam 2- Volume to surface, or volume 3- Beam to surface Table to surface, volume or beams
8	Usability and Productivity
	The software should have the following features to execute an efficient, automatable, and extensible simulation framework. 1- Customized user interaction elements for setting up the simulation. 2- A fully inbuilt tool to compare side-by-side two simulation setups or files to identify the differences. 3- Support a "general expression" type of language through which users can provide custom scalar, vector, or tensor functions that vary in space and with time without any prior knowledge of a programming language. The editor to write these functions is fully integrated into the software and the editor supports predictive typing, auto-complete based on selection, and provides a preview panel to see the behaviour of custom functions or fields. 4- Provide a framework to parameterize the important elements of simulation setup through user-defined, spatially invariant scalar, and vector constants. These parameters should support file paths and is reference able in user-written functions that can be plugged into any



expression.

- 5- The software should provide an inbuilt method to writing user queries (logic-based) to sub-select certain entities within the simulation setup robustly. These should be built using conditional statements and support Boolean operators both in un-nested and nested forms.
- 6- The software should facilitate building a blank "Template" file through which a simulation can be quickly setup without much user intervention.
- 7- A framework to execute primitive workflows automatically without any need for scripting, programming, or any textual command passing methods.
- 8- The software client GUI is to be based on JAVA and can record user interface actions in a JAVA based script that can be edited, adapted, and played back freely to execute any custom-built workflows or methods. The JAVA script and supported API should incorporate complex algorithms and routines for automation. The libraries should be freely available so that they can be used in an IDE environment for creating or editing scripts.

9. ACCEPTANCE TEST PLAN

1. The analysis software should demonstrate CFD workflow process using a single file leveraging unlimited HPC cores for solving
2. The software's environment should offer all stages of engineering analysis within a single graphical user interface
 - Import and creation of geometries that are simple and complex in their topologies.
 - Edit imported geometries using either solid body operation or surface modelling.
 - Ability to generate structured and unstructured meshes with different cell types and topologies.
 - The solution of the governing equations for a specific class of problem on UNLIMITED HPC cores with a single license.
 - Analysis of the simulation results.
 - Automation of the simulation workflows using different techniques not limited to scripting.
 - Connection to other CAE software for co-simulation analysis.
3. The software environment should have an automated methodology to include a multiple time-scale(CHT)workflow in a single simulation.
4. The software environment should be able to perform solution/model based adaptive mesh refinement AMR for multi-physics simulation such as VOF, Reactive Flows, Overset meshes without use of scripting macros/journals.
5. The software environment should allow adjoin based simulation to compute sensitivity of the objective (output) with respect to the design variables (input).
6. The software environment should allow in single graphical interface provide simulation capabilities for electromagnetic simulations.
7. The software should be able to perform optimization studies in the same workflow and offer unique search algorithm— such that it performs a Simultaneous Hybrid Exploration that is Robust, Progressive, and Adaptive.
8. The software environment should allow in a single graphical interface provide simulation capabilities build electric circuits to



investigate the effect of circuit component choices on the electromagnetic performance.

9. The software environment should allow leveraging CAE software for co-simulation analysis that can be performed through FMI.
10. The software environment should have Reduced Order Model (ROM) capability to create images from CFD to mathematical model for visualization and also converting any high-fidelity simulations, test data into reusable mathematical models for real time applications and predictive maintenance.
11. The software environment should allow modelling real gas like effects and provide libraries for modelling nozzles with $Ma > 5$.
12. The software environment should allow to view the results seamlessly from the solution file, in existing Virtual Reality (VR) hardware's, with no additional license features.
13. Showcase software capability on store separation problem.

