Consulting Fire Engineers
34 Satara Crescent
Khandallah
Wellington 6035
New Zealand

FDS 6.7.1

Verification Report

on the

FireNZE Linux IB Cluster

Prepared by: FireNZE

Dated: 1 September 2019

Revision: R01

Table of Contents

1 Executive Summary

FireNZE has completed a verification study of Fire Dynamics Simulator (FDS) Version 6.7.1 on our Linux Cluster in accordance with the Verification Suite specified in Appendix B of the FDS Verification Guide[1].

The study was warranted because of an FDS version upgrade from FDS 6.7.0.

FDS parallel processing was tested is accordance with Section 3 of the FDS Users Guide[3] using MPI and OMP.

- The FireNZE installation of FDS Version 6.7.1 complies with the verification criteria of the NIST Verification Suite.

- The cluster is fully functional, stable and robust for extended processing times.

- The cluster demonstrates effective MPI and OMP scaling.

- The FireNZE cluster provides comparable processing speed to previous FDS installations, and is significantly faster than benchmarked commercial High Performance Computer (HPC) resources for identical model and process allocations.

2 Introduction

2.1 Verification

Verification is the process of testing the installation of FDS executable files on a particular computational platform through a comparison of the output from prescribed FDS models[1] against expected output and tolerances.

Expected outputs and tolerances for FDS have been established by the National Institute of Science and Technology (NIST) in Appendix A of Reference 1.

Every FDS installation should be verified, whether the installation is completed from pre-compiled binaries or compiled source code, in order to provide a minimum level of confidence that FDS operates as intended on the installation computational domain (hardware and software).

It should be noted that:

- it is impossible to test every aspect of FDS.
- it is prohibitively time consuming to test every computational node under every available process allocation on a large cluster.
- some FDS models may fail to run or result in numerical instability even though the program has been verified.
- verification does not ensure the appropriateness of the FDS program or of a particular FDS model for the intended application.
- a given FDS model on a particular hardware and software platform with identical process allocations will always produce identical results.

The applied verification suite is a minimum set of FDS models for quality assurance of an FDS installation as specified in Appendix B of Reference 1. Other verification tests may be warranted subject to specific user modelling requirements. A comprehensive list of extended verification tests is contained in Appendix A of Reference 1.

This verification study is based on point measurements at specific instances in time however many of the metrics are time variant. In this study a number of metrics have been graphed as time histories and visually examined for gross transients or discrepancies (a qualitative analysis). A quantitative analysis can be completed at discrete time steps and/or by comparison of areas under curves through numerical integration.

2.2 Validation

The appropriateness of FDS to simulate fire phenomena is determined by validation. Every release version of FDS has been validated by NIST[2]. Validation is independent of the computational environment.

2.3 Parallel Processing

FDS verification does not consider parallel processing using MPI and/or OMP. The verification models were run as a single and dual MPI process with between one and four OMP threads for best batch processing of concurrent models.

Parallel processing was tested for gross errors (program fault or computational error) with MPI and OMP performance tests using a FireNZE standard model. These tests provide a measure of parallel processing performance with increasing allocation of parallel computational resources.

2.4 Processing Speed

Processing speed is not easily defined because it depends on hardware, software, resource allocation, and the FDS test model.

FireNZE uses a standard compartment fire model specifically developed to test typical fire modelling parameters often used in commercial fire engineering modelling for the built environment.

NIST specifies its own computational processing benchmark models in Appendix A of Reference 1. The NIST openmp_test128x.fds model time stepping wall clock time is reported.

3 Linux Platform

The following is a general description of the FireNZE Linux Cluster computational environment.

Any significant changes to the computational environment may warrant re-verification of FDS.

3.1 Hardware

The hardware is a Beowulf cluster built by FireNZE as a low-cost dedicated solution for fast processing of a limited number of FDS models with moderate parallelization (with up to 26 physical cores per model).

The cluster comprises four Intel I7 4097K quad core processor nodes, each with a turbo clock speed of 4.4 GHz, 16 GB RAM, solid state and conventional hard drives, connected with a dedicated 40 Gb/s Infiniband network and 1 Gb/s Ethernet backplane. A further node has been implemented with an Intel I9 7900X processor with a turbo clock speed of 4.5 GHz, 24 GB RAM, with solid state and conventional hard drives.

The Linux cluster is connected via 1 Gb/s Ethernet to a Windows 10 workstation with an I9-9900K 8 core processor with a turbo clock speed of 4.8 GHz. This node is used for model development and analysis using the NIST compiled FDS 6.7.1 bundle For Windows. This resource is not generally used for commercial modeling and is verified on an as required basis.

3.2 Software

3.2.1 Operating System

Ubuntu 16.04.1 LTS, 64 bit, kernel 4.4.0-104-generic.

3.2.2 FDS

Fire Dynamics Simulator (FDS) Version 6.7.1 for Linux 64 bit platforms compiled by FireNZE using Intel Fortran (Intel Parallel Studio XE 2018) with processor specific optimizations and the Intel Maths Kernel Library (MKL).

3.2.3 MPI

Intel MPI (Intel Parallel Studio XE 2018 Cluster Edition).

3.2.4 OFED

Mellanox 3.4-2.0.0.0 for Linux compiled under GNU Fortran 5.5

4 Method

4.1 Verification

The prescribed FDS models were run on the Linux cluster with between one and four allocated OMP threads for best batch processing efficiency. The resulting model metrics were compared with prescribed point values and tolerances resulting in either a Pass or Fail.

4.2 Parallel Processing Study

Both MPI and OMP were tested using FireNZE's standard compartment fire model assigned across various nodes and utilizing between 1 to 4 OMP threads and 1 to 16 MPI processes.

4.3 Processing Speed

FireNZE compares the performance of other FDS platforms and versions with the current installation using historical performance records based on FireNZE's standard compartment fire model. These tests are comparative rather than definitive.

5 Results

5.1 Verification

The verification results are presented in Appendix A.

All point metrics with within prescribed tolerances for expected values.

5.2 Parallel Processing Performance

The High Performance Computer (HPC) models[4] developed by FireNZE for comparative performance tests were run to completion using 1, 2, 4, 8 and 16 MPI processes with 1, 2 and 4 OMP threads to node slot limits.

The models all ran to completion without gross error. This test suite provided over 62 core hours of continuous processing demonstrating that the platform is robust for commercial applications.

5.2.1 OMP Scaling

OMP scaling is effective as shown in Figure 1. The best performance increase is with a limited increase in scaling from one to two OMP threads. Increased OMP scaling beyond two threads leads to reduced processing speed returns for allocated computational resources and, in general, overall processing speed will be increased by running concurrent models above two OPM threads.

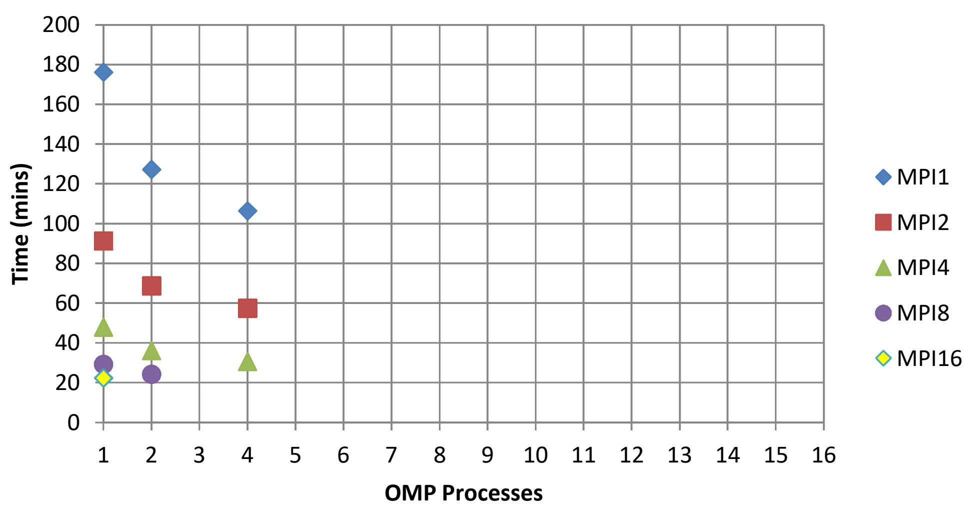

Figure 1. FDS 6.7.1 Simulation Time with Increasing OMP Parallelization
260K Computational Domain, Model M10-xx.fds

5.2.2 MPI

MPI scaling is effective as shown in Figure 2. MPI generally offers a better performance increase than OMP as evident from the projected slope of Figures 1 and 2.

MPI scaling is most effective to four MPI processes. Increased MPI scaling beyond four processes leads to reduced processing speed returns and, in general, overall processing efficiency will be increased by running concurrent models rather than allocating more MPI processes.

When allocating slots better performance will be obtained by avoiding full node subscriptions.

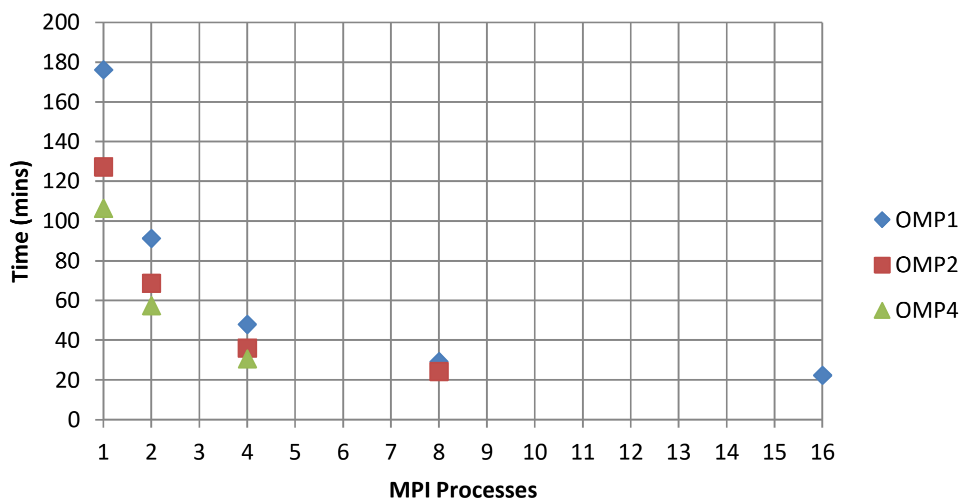

Figure 2. FDS 6.6.0 Simulation Time with Increasing MPI Parallelization
260K Computational Domain, Model M10-xx.fds

5.2.3 Processing Speed

The relative speed of the FDS 6.7.1 upgrade compared with previous FDS installations and other platforms for the M10-xx model is shown in Figure 3. This test indicates that the processing speed of FDS 6.7.1 on the FireNZE cluster is comparable to previous installations.

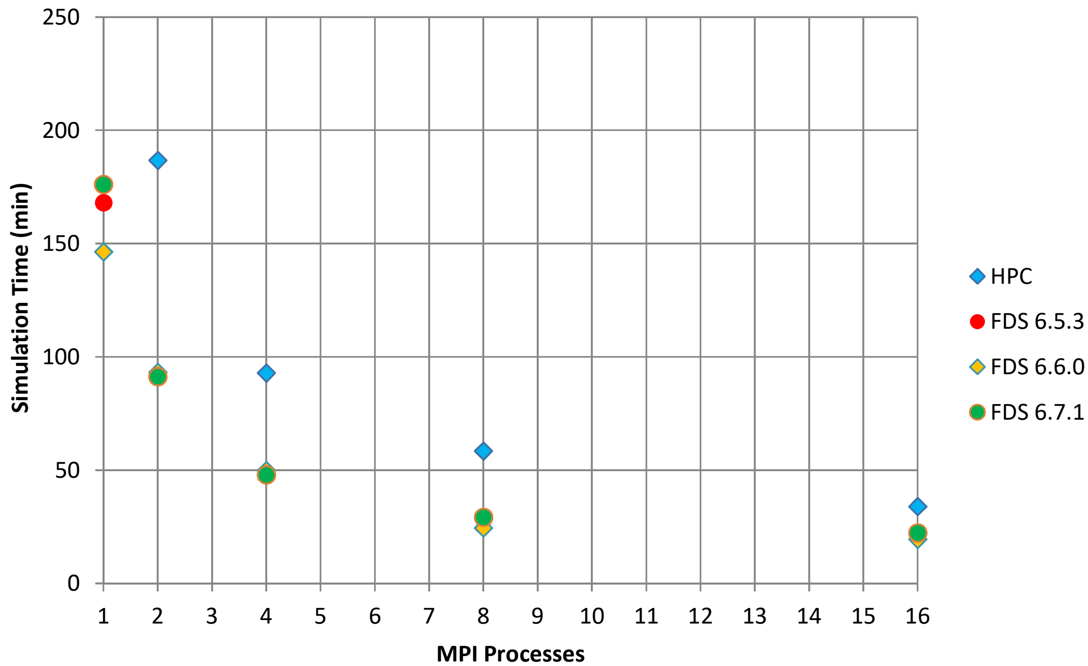

Figure 3. Simulation Time between Installations
260K Computational Domain, Model M10-xx.fds

The processing speed of the NIST openmp_test128x.fds model with 4 OMP processes on node Slave0 was 234 seconds Time Stepping Wall Clock Time. This is comparable with FDS 6.6.0 and 6.7.0.

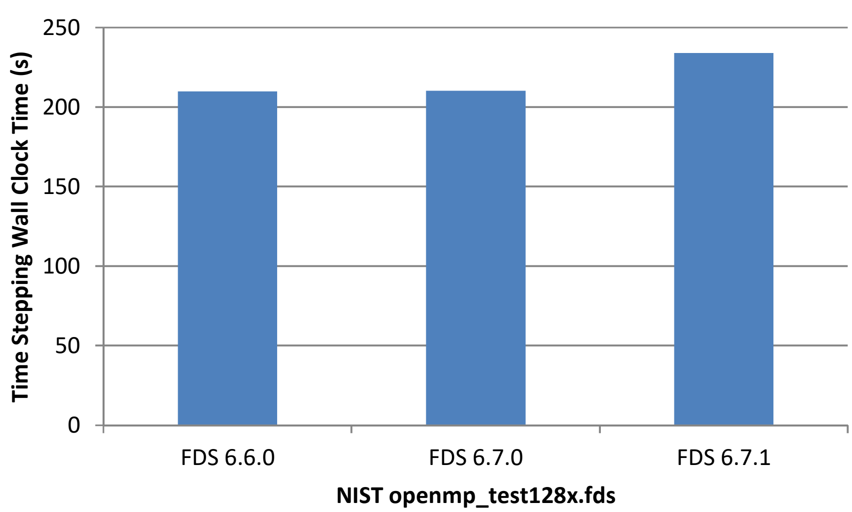

Figure 4. Simulation Time of NIST openmp_test128x.fds
(4 OMP processes on node Slave0)

6 Conclusions

The FDS 6.7.1 installed on the FireNZE Linux cluster:

- compiles with the NIST minimum verification suite.
- is robust under MPI and OMP with good scaling.
- provides comparable processing speed against historical benchmarks.

(Original signed by)

T.G. O'Brien, PG Cert. Eng. (Fire), BE(Hons.), MSFPE, MNFPA, CMEngNZ, Int. PE
Consulting Fire Engineer
FireNZE (a trading division of Aquacoustics Limited)

1 September 2019

7 References

1. National Institute of Standards and Technology (NIST), Special Publication 1018-2, Fire Dynamics Simulator Technical Reference Guide Volume 2: Verification, 6th Ed., FDS Ver. 6.5.0, 22 June 2016, Rev. Git-r14-0-gec73757, U.S. Department of Commerce

2. National Institute of Standards and Technology (NIST), Special Publication 1018-3, Fire Dynamics Simulator Technical Reference Guide Volume 2: Validation, 6th Ed., FDS Ver. 6.5.0, 22 June 2016, Rev. Git-r14-0-gec73757, U.S. Department of Commerce

3. National Institute of Standards and Technology (NIST), Special Publication 1019, Fire Dynamics Simulator User's Guide, 6th Ed., FDS Ver. 6.5.0, 22 June 2016, Rev. Git-r14-0-gec73757, U.S. Department of Commerce

4. T.G. O'Brien, High Performance Computing as a Resource for Fire Engineering Design, FireNZE, 26 April 2016

Appendix A Verification Summary

FDS 6.7.1 Verification 1 September 2019

Test	FDS Model	Output File	Metric	Units	Measurement Time	Predicted (Model) Value	Expected Value	Type of Error	Error	Error Tolerance	Pass/Fail	Margin
Controls	activate_vents.fds	activate_vents_ctrl.csv	controller_1	Logic	3.00E+00	1.0000E+00	1.00E+00	Relative	0.00E+00	0.00E+00	Pass	
			controller_3	Logic	8.10E+00	1.0000E+00	1.00E+00	Relative	0.00E+00	0.00E+00	Pass	
			controller_4	Logic	1.20E+01	1.0000E+00	1.00E+00	Relative	0.00E+00	0.00E+00	Pass	
Pressure Effects	isentropic2.fds	isentropic2_devc.csv	density_1	kg/m3	6.00E+02	1.3645E+00	1.36E+00	Relative	3.35E-03	1.00E-02	Pass	33
			density_2	kg/m3	6.00E+02	1.3645E+00	1.36E+00	Relative	3.35E-03	1.00E-02	Pass	33
			pressure_1	Pa	6.00E+02	6.29E+04	6.29E+04	Relative	-6.03E-04	3.00E-02	Pass	2
			pressure_2	Pa	6.00E+02	6.3974E+04	6.40E+04	Relative	-4.07E-04	3.00E-02	Pass	1
			temperature_1	C	6.00E+02	1.3390E+02	1.34E+02	Relative	-7.20E-04	3.00E-02	Pass	2
			temperature_2	C	6.00E+02	1.35E+02	1.35E+02	Relative	1.96E-03	3.00E-02	Pass	7
			enthalpy_1	kJ/m3	6.00E+02	5.7465E+02	5.75E+02	Relative	-6.00E-04	1.00E-02	Pass	6
			enthalpy_2	kJ/m4	6.00E+02	5.7855E+02	5.79E+02	Relative	-7.83E-04	1.00E-02	Pass	8
Energy Budget	energy_bugdet_tmix.fds	energy_bugdet_tmix_devc.csv	temp	C	2.00E+01	1.0000E+02	1.00E+02	Relative	1.35E-05	1.00E-02	Pass	0
Energy Budget	energy_bugdet_cold_walls.fds	energy_bugdet_cold_walls_hrr.csv	Q_DIFF	kW	6.00E+02	-7.8806E-02	2.70E+00	Absolute	-2.78E+00	1.20E+01	Pass	23
Fires	spray_burner.fds	spray_burner_hrr.csv	*	kJ	*	7.9773E+04	7.98E+04	Relative	-3.35E-04	5.00E-02	Pass	1
Heat Transfer	heat_conduction_kc.fds	heat_conduction_kc_devc.csv	cart_front	C	1.00E+03	1.5841E+02	1.58E+02	Relative	2.57E-03	1.00E-02	Pass	26
			cyl_front	C	1.00E+03	1.8209E+02	1.82E+02	Relative	4.69E-04	1.00E-02	Pass	5
			sph_front	C	1.00E+03	2.0953E+02	2.10E+02	Relative	-2.23E-03	1.00E-02	Pass	22
			cart_back	C	1.00E+03	4.9517E+00	4.98E+00	Relative	4.41E-03	2.00E-02	Pass	22
			cyl_back	C	1.00E+03	1.9780E+01	1.98E+01	Relative	-1.01E-03	2.00E-02	Pass	5
			sph_back	C	1.00E+03	4.4877E+01	4.48E+01	Relative	1.72E-03	2.00E-02	Pass	9
HVAC	ashrae7_table.fds	ashrae7_table_devc.csv	Duct 1	Pa	3.00E+01	7.1431E+02	7.16E+02	Relative	-2.63E-03	1.02E+00	Pass	0
			Duct 2	Pa	3.00E+01	4.4008E+02	4.41E+02	Relative	-2.54E-03	2.02E+00	Pass	0
			Duct 3	Pa	3.00E+01	4.4008E+02	4.41E+02	Relative	-2.54E-03	3.02E+00	Pass	0
			Duct 4	Pa	3.00E+01	2.7425E+02	2.75E+02	Relative	-2.73E-03	4.02E+00	Pass	0
			Duct 5	Pa	3.00E+01	1.2095E+02	1.21E+02	Relative	-2.89E-03	5.02E+00	Pass	0
			Duct 56	Pa	3.00E+01	7.2876E+02	7.31E+02	Relative	-3.19E-03	6.02E+00	Pass	0
			Duct 6	Pa	3.00E+01	3.2110E+01	3.22E+01	Relative	-2.80E-03	7.02E+00	Pass	0
			Duct 7	Pa	3.00E+01	3.1202E+02	3.13E+02	Relative	-3.78E-03	8.02E+00	Pass	0
Pressure Solver	duct_flow.fds	duct_flow_devc.csv	flow_out	m3/s	6.00E+01	9.9520E-01	1.00E+00	Relative	-4.80E-03	5.00E-02	Pass	10
Pyrolysis	enthalpy.fds	enthalpy_devc.csv	T_slab	C	7.00E+00	1.5575E+02	1.56E+02	Relative	-1.63E-03	1.00E-02	Pass	16
Pyrolysis	shrink_swell.fds	shrink_swell_devc.csv	M_1	kg/m2	1.50E+01	5.0000E-01	5.00E-01	Relative	0.00E+00	1.00E-02	Pass	0
			M_4	kg/m2	1.50E+01	1.0000E+00	1.00E+00	Relative	0.00E+00	1.00E-02	Pass	0
			L_1	m	1.50E+01	5.0000E-04	5.00E-04	Relative	0.00E+00	1.00E-02	Pass	0
			L_4	m	1.50E+01	2.0000E-03	2.00E-03	Relative	0.00E+00	1.00E-02	Pass	0
Radiation	radiation_shield.fds	radiation_shield_devc.csv	Flux	kW/m2	4.00E+02	4.7622E+00	4.76E+00	Relative	4.62E-04	1.00E-02	Pass	5
			Temp	C	4.00E+02	3.8032E+02	3.80E+02	Relative	8.49E-04	1.00E-02	Pass	8
Species	reactionrate_EDC_1step_CH4_nonmix.fds	reactionrate_EDC_1step_CH4_nonmix_devc.csv	TEMP	C	6.00E+01	2.4844E+03	2.47E+03	Relative	5.83E-03	1.00E-02	Pass	58
			PRES	Pa	6.00E+01	8.3582E+05	8.34E+05	Relative	2.18E-03	1.00E-02	Pass	22
Species	reactionrate_arrhenius_2order_1step.fds	reactionrate_arrhenius_2order_1step_devc.csv	O2	kg/kg	5.00E+00	1.3233E-02	1.30E-02	Absolute	2.33E-04	1.00E-03	Pass	23
			C3H8	kg/kg	5.00E+00	3.2891E-03	3.36E-03	Absolute	-7.09E-05	1.00E-03	Pass	7
			CO2	kg/kg	5.00E+00	1.6980E-01	1.70E-01	Absolute	-2.00E-04	1.00E-03	Pass	20
			H2O	kg/kg	5.00E+00	9.2677E-02	9.27E-02	Absolute	-2.30E-05	1.00E-03	Pass	2
Sprinklers and Sprays	water_evaporation_1.fds	water_evaporation_1_devc.csv	humid	%	1.00E+01	2.1097E+00	2.11E+00	Relative	-1.48E-04	1.00E-02	Pass	1
			h_gas	kJ	1.00E+01	-1.6664E+02	-1.67E+02	Relative	-2.15E-03	1.00E-02	Pass	22
			h_water	kJ	1.00E+01	1.5887E+02	1.59E+02	Relative	-8.22E-04	1.00E-02	Pass	8
			dens	kg/m3	1.00E+01	1.0000E-02	1.00E-02	Relative	0.00E+00	1.00E-02	Pass	0
			Temp	C	1.00E+01	1.5436E+02	1.54E+02	Relative	2.32E-03	1.00E-02	Pass	23
			pres	Pa	1.00E+01	-7.8013E+03	-7.81E+03	Relative	-1.11E-03	1.00E-02	Pass	11
		water_evaporation_1_mass.csv	WATER VAPOR	kg	1.00E+01	1.0000E-02	1.00E-02	Relative	0.00E+00	1.00E-02	Pass	0
Sprinklers and Sprays	particle_drag_U50_N16.fds	particle_drag_U50_N16_devc.csvs	U-VEL	m/s	5.00E+01	2.9931E+00	2.99E+00	Absolute	3.14E-03	1.00E-02	Pass	31

* Derived from HRR: SUM(HRR*del t) - (HRR90 + HRR0)/2