

1 Scenario: Balanced Workload

Table 1: Balanced scenario results on Snellius

Subdomain Size [μm]	H	Result [S]	Prediction [S]	Prediction Error [%]
(25.0, 12.5, 12.5)	0%	12.84 ± 0.29	13.19	2.69
	9%	14.93 ± 0.26	14.73	1.29
	10%	15.37 ± 0.28	15.04	2.11
	12%	15.86 ± 0.36	15.35	3.18
	14%	15.29 ± 0.32	15.66	2.44
	16%	16.78 ± 0.35	15.97	4.85
	18%	17.08 ± 0.33	16.28	4.70
(50.0, 50.0, 25.0)	0%	136.67 ± 3.28	122.39	10.45
	9%	160.98 ± 3.34	147.10	8.62
	10%	166.87 ± 4.08	152.04	8.88
	12%	169.65 ± 3.47	156.99	7.47
	14%	174.50 ± 3.38	161.93	7.21
	16%	180.06 ± 4.01	166.87	7.32
	18%	186.50 ± 3.98	171.81	7.87
(50.0, 50.0, 50.0)	0%	238.40 ± 0.60	230.61	3.27
	9%	281.36 ± 0.51	280.04	0.47
	10%	288.36 ± 0.46	289.92	0.54
	12%	300.60 ± 6.73	299.81	0.27
	14%	307.00 ± 0.41	309.69	0.88
	16%	315.93 ± 0.41	319.58	1.15
	18%	329.38 ± 0.66	329.46	0.03
(50.0, 100.0, 50.0)	0%	470.81 ± 7.74	447.06	5.04
	9%	562.62 ± 11.82	545.91	2.97
	10%	579.01 ± 11.65	565.68	2.30
	12%	590.62 ± 2.54	585.45	0.88
	14%	608.66 ± 1.53	605.22	0.57
	16%	626.35 ± 2.79	624.99	0.22
	18%	654.80 ± 13.90	644.76	1.53

Table 2: Balanced scenario results on DAS6

Subdomain Size [μm]	H	Result [S]	Prediction [S]	Prediction Error [%]
(12.5, 25.0, 25.0)	0%	13.68 ± 0.02	15.34	12.11
	9%	15.62 ± 0.07	17.01	8.90
	10%	15.37 ± 0.03	17.35	12.87
	12%	16.29 ± 0.05	17.68	8.51
	14%	16.11 ± 0.02	18.02	11.81
	16%	17.17 ± 0.14	18.35	6.88
	18%	17.14 ± 0.02	18.68	9.02
(25.0, 25.0, 25.0)	0%	23.25 ± 0.03	24.43	5.08
	9%	27.55 ± 0.10	28.01	1.67
	10%	27.27 ± 0.03	28.73	5.34
	12%	28.93 ± 0.08	29.44	1.80
	14%	28.73 ± 0.05	30.16	5.00
	16%	30.41 ± 0.02	30.88	1.52
	18%	30.50 ± 0.05	31.59	3.60
(50.0, 50.0, 50.0)	0%	149.74 ± 0.16	148.73	0.67
	9%	175.02 ± 0.08	177.40	1.36
	10%	179.34 ± 0.23	183.13	2.12
	12%	186.45 ± 1.55	188.87	1.30
	14%	190.67 ± 0.08	194.60	2.06
	16%	196.32 ± 0.17	200.33	2.04
	18%	203.20 ± 0.18	206.07	1.41
(50.0, 100.0, 50.0)	0%	298.43 ± 2.53	289.46	3.01
	9%	349.15 ± 0.03	346.79	0.68
	10%	358.06 ± 0.23	358.26	0.05
	12%	369.29 ± 0.35	369.72	0.12
	14%	380.30 ± 0.17	381.19	0.23
	16%	391.14 ± 0.20	392.65	0.39
	18%	404.36 ± 0.28	404.12	0.06

2 Scenario: Imbalanced Subdomains

Table 3: Subdomain imbalance scenario results. In the balanced configuration, each process is assigned a (50, 50, 50) μm subdomain. For the imbalanced configuration half the processes are responsible for 75% of the domain. Each configuration is run for 500 iterations, the average and standard deviation of three runs are reported. Each run utilizes all available hardware threads in a single node of the targeted machine, 128 on Snellius and 24 on DAS6.

Machine	RBCs	Balanced Results [s]	Imbalanced Results [s]	Balanced Prediction [s]	Balanced Prediction Error [%]	Imbalanced Prediction [s]	Imbalanced Prediction Error [%]
das6	00%	149.74 ± 0.16	222.61 ± 1.06	148.73	0.67	235.12	5.62
das6	18%	203.20 ± 0.18	343.14 ± 0.41	206.07	1.41	321.11	6.42
snellius	00%	238.40 ± 0.60	422.92 ± 0.31	230.61	3.27	367.17	13.18
snellius	18%	329.38 ± 0.66	612.37 ± 7.96	329.46	0.03	515.44	15.83

3 Scenarios: Imbalanced Hematocrit

Table 4: Hematocrit imbalance scenario results. The reported results and predictions are excluding the fluid computation. Each configuration is run for 500 iterations with a subdomain size of (50, 50, 50) μm , the average and standard deviation of 3 runs are reported. Each experiment utilizes all available hardware threads on a single node of the targeted machine, 128 on Snellius and 24 on DAS6.

Machine	RBCs	Distribution [Processes]	Balanced RBCs	Balanced Results [s]	Imbalanced Results [s]	Balanced Prediction [s]	Balanced Prediction Error [%]	Imbalanced Prediction [s]	Imbalanced Prediction Error [%]
das6	9%	12 / 12	14%	46.78 \pm 0.39	56.83 \pm 0.09	47.57	1.68	59.04	3.88
das6	0%	12 / 12	9%	29.01 \pm 0.18	54.35 \pm 0.31	30.37	4.69	59.04	8.61
snellius	9%	16 / 112	10%	58.89 \pm 1.92	88.71 \pm 1.03	64.08	8.81	103.62	16.80
snellius	0%	16 / 112	2%	13.66 \pm 0.49	81.67 \pm 0.81	12.42	9.07	103.62	26.87
snellius	9%	64 / 64	14%	80.47 \pm 0.97	98.21 \pm 0.91	83.85	4.19	103.62	5.50
snellius	0%	64 / 64	9%	49.08 \pm 1.30	96.72 \pm 0.56	54.19	10.42	103.62	7.13

4 Scenario: Imbalanced Communication

Table 5: Communication-imbalance scenario results on Snellius. Each configuration is run for 500 iterations with a subdomain size of (50, 50, 50) μm , the average and standard deviation of 3 runs are reported. Each experiment utilizes all available hardware threads, 128 on Snellius.

RBCs	Distribution [Processes]	Fluid Ratio	Particle Ratio	Imbalanced Results [s]	Old Prediction [s]	Old Prediction Error [%]	Updated Prediction [s]	Updated Prediction Error [%]
0%	8 / 120	5/18	5/26	264.55 \pm 0.42	329.46	24.53	303.19	14.60
9%	8 / 120	12/18	8/26	280.04 \pm 0.50	329.46	17.65	314.64	12.36
0%	16 / 112	8/18	8/26	265.64 \pm 0.93	329.46	24.03	308.65	16.19
9%	16 / 112	12/18	8/26	282.39 \pm 0.71	329.46	16.67	314.64	11.42
0%	32 / 92	12/18	16/26	283.50 \pm 4.75	329.46	16.21	317.24	11.90
9%	32 / 92	18/18	13/26	295.25 \pm 5.11	329.46	11.59	325.24	10.16