Supplementary File of the paper “NAIMEO: Niching Area and Inverse Model-Based Evolutionary Optimizer to Solve Multi-modal Multi-objective Optimization Problems”

I. NOTATIONS AND ACRONYMS

We list all the acronyms and their full names, as well as important symbols and their definition in table S-I and S-II, respectively.

TABLE S-I
ALL THE ACRONYM AND THEIR FULL NAMES

Acronym	Full name
MMOP	Multimodal Multi-objective Optimization Problem
MMEA	Multimodal Multi-objective Evolutionary Algorithms
MOEAs	Multi-Objective Evolutionary Algorithm
PS	Pareto Set
PF	Pareto Front
IMEA	Inverse Model- Assisted Evolutionary Algorithm
FE	Fitness Evaluation
IGD	Inverted Generation Distance
IGDX	Inverted Generation Distance in Decision Space
PSP	Pareto Sets Proximity
EA	Evolutionary Algorithm
s	K-Nearest Neighbor

TABLE S-II
ALL THE IMPORTANT SYMBOLS AND THEIR DEFINITION

Notation	Definition
$b \preccurlyeq a$	b dominates a
$b \preccurlyeq^{\epsilon} a$	b ϵ-dominates a
$d^{obj}(\cdot)$	Euclidean distance in objective space
$d^{dec}(\cdot)$	Euclidean distance in decision space
$\hat{d}$	a mean distance value for $\widehat{N}$
$dist(a, a^{obj})$	Euclidean distance in objective space between a and its nearest neighbor in P
$dist(a, a^{dec})$	Euclidean distance in decision space between a and its nearest neighbor in P
D	number of decision variable
D_a	diversity assessment for solution a
$\widehat{D}_a$	representation of the diversity in objective space
$\breve{D}_a$	representation of the diversity in decision space
$\boldsymbol{f}(\cdot)$	multi-objective functions to be optimized
$\hat{G}$	the number of groups
$\breve{G}$	the length for a single group
M	number of objective functions
$\tilde{\tilde{n}}$	the number of equivalent Pareto sets
N	size of population
$\widehat{N}$	a solution set that rank at the first level in non-dominated solution sorting
N_d	number of disturbances in decision variable analysis
NR_x	number of solutions that dominates s_x
$\widetilde{N}_x$	the fitness value for environmental selection of multi-modal optimization
P	population
P_a	convergence assessment for solution a
$p^{\epsilon}(a, b)$	ϵ-Pareto dominance
$\boldsymbol{R}^*$	a solution randomly chosen from population
$rescale(\cdot)$	a range-restricted function that unifies the distance values
$\boldsymbol{s^i}$	i-th solution of $\widehat{N}$
$\boldsymbol{s^{i^*}}$	the closest neighbor to $\boldsymbol{s^i}$ in objective space
$\boldsymbol{s^{i^\wedge}}$	the closest neighbor to $\boldsymbol{s^i}$ in decision space
S^*	a set of solutions with a uniform distribution on the true Pareto solution set
S	a solution set derived from an algorithm
T	a linear inverse model
V_O	multi-objective optimization related variables
V_M	multi-modal optimization related variables
$\hat{x}^{i,*}$	the maximum value of the i-th decision variable of S^*
$\breve{x}^{i,*}$	the minimum value of the i-th decision variable of S^*
$\hat{x}^{i}$	the maximum value of the i-th decision variable of S
$\breve{x}^{i}$	the minimum value of the i-th decision variable of S
$\boldsymbol{x}$	a decision vector
X	the decision matrix
Y	the objective matrix
$\boldsymbol{\pi}(\cdot)$	an inverse modeling function
Ω	a 2 by 2 matrix
$D_o(\cdot)$	the value for superior solution selection
$\sigma(\cdot)$	an activation function

II. ADDITIONAL EXPERIMENTAL RESULTS

We give more information about our algorithm and additional results. The flowchart NAIMEO is shown in Fig. S-1.

As shown in Table S-III and S-IV, we give IGDX and 1/PSP values to fully assess algorithms’ performance in decision space. Just for 1/PSP values, NAIMEO surpasses HREA, HHC-MMEA, CoMMEA, CMMO and MMEAPSL by 19, 16, 17, 16 and 17. IGD values on instances with 500 and 1000 decision variables with 4 and 8 equivalent Pareto sets are summarized statistically in Table S-V, and IGDX is shown in Table S-VI. From them, we can see NAIMEO exceeds HHC-MMEA in most cases.

The convergence curves of the IGD values of all algorithms on 5-objective 10-dimensional MMMOP1-6 problems are displayed in Fig. S-2 to completely illustrate the efficacy of all algorithms. NAIMEO's superior performance in terms of efficiency and convergence in comparison with its peers are well shown.

We provide a distribution of the obtained solutions from NAIMEO and HHC-MMEA in objective and decision spaces, as shown in Fig. S-3 and S-4. From them, we can see that HHC-MMEA cannot converge to the true Pareto Front in a half of the cases, whereas NAIMEO can reach an even distribution in true PFs with 5 out of 6 cases. Besides, NAIMEO can cover more real Pareto Sets than HHC-MMEA do.

TABLE S-III

IGDX VALUES OF THREE ALGORITHMS ON MMMOPS AND SMMOPS, WHERE BEST RESULTS ON EACH TEST INSTANCE ARE IN BOLD

Problem	*M*	*D*	HREA	HHC-MMEA	CoMMEA	CMMO	MMEAPSL	NAIMEO(ours)
MMMOP1	3	10	1.1644E+00(4.05E-01) −	5.8100E-01(3.10E-02) −	8.0510E-01(6.13E-02) −	5.4686E-01(4.23E-02) −	7.8051E-01(3.16E-02) −	**4.2604E-01(3.01E-02)**
	5	10	1.0506E+00(3.22E-01) −	9.6332E-01(3.57E-02) −	8.1988E-01(5.18E-02) −	4.9072E-01(7.12E-02) −	6.0373E-01(4.27E-02) −	**4.8397E-01(4.81E-02)**
MMMOP2	3	10	1.0910E+00(5.01E-01) −	2.7337E-01(5.02E-02) −	1.4635E-01(3.76E-02) +	**1.0841E-01(9.51E-02)** +	1.2505E-01(9.52E-02) +	2.2133E-01(4.57E-02)
	5	10	1.0387E+00(7.31E-01) −	3.7132E-01(4.83E-02) +	9.3735E-01(5.18E-02) −	3.5628E-01(4.26E-02) −	4.5223E-01(3.44E-02) −	**2.8464E-01(3.15E-02)**
MMMOP3	3	10	9.6328E-01(8.76E-02) −	3.1597E-01(5.96E-02) −	2.7350E-01(4.33E-02) −	1.5766E-01(1.51E-02) −	**1.2346E-01(4.55E-02)** +	1.3549E-01(4.72E-02)
	5	10	1.1084E+00(2.50E-01) −	6.9877E-01(2.89E-02) −	8.3810E-01(1.03E-02) −	4.9020E-01(3.12E-02) −	5.6311E-01(7.26E-02) −	**3.9041E-01(6.08E-02)**
MMMOP4	3	10	1.1492E+00(3.48E-01) −	7.0075E-01(5.45E-02) −	7.0108E-01(1.56E-02) −	7.0393E-01(2.37E-02) −	8.3863E-01(6.12E-02) −	**4.0421E-01(2.56E-02)**
	5	10	1.1461E+00(2.74E-01) −	9.1012E-01(9.03E-02) −	1.0781E+00(4.02E-01) −	6.6599E-01(1.99E-02) −	7.4320E-01(5.65E-02) −	**4.7599E-01(2.96E-02)**
MMMOP5	3	10	1.1924E+00(6.27E-01) −	**4.5005E-01(8.15E-02)** ≈	7.9849E-01(5.27E-02) −	5.7213E-01(1.27E-02) −	7.3589E-01(8.17E-02) −	4.5778E-01(4.66E-02)
	5	10	1.2051E+00(2.55E-01) −	9.8715E-01(3.60E-02) −	1.1598E+00(7.92E-01) −	5.9007E-01(3.97E-02) −	7.9260E-01(8.43E-02) −	**5.0351E-01(1.40E-02)**
MMMOP6	3	10	1.1361E+00(4.66E-01) −	9.2485E-01(8.82E-02) +	**9.0439E-01(5.15E-02)** +	9.9725E-01(2.75E-02) ≈	1.0026E+00(5.17E-01) ≈	1.0168E+00(6.12E-01)
	5	10	9.0364E-01(1.44E-02) −	8.7702E-01(5.05E-02) −	**6.8684E-01(8.44E-02)** +	6.9226E-01(3.37E-02) +	7.7239E-01(1.67E-02) +	8.5793E-01(1.87E-02)
SMMOP1	3	100	1.2948E+01(4.35E+00) −	1.9051E+00(1.10E-01) −	4.1828E+00(2.40E-01) −	4.1272E+00(7.10E-01) −	3.9848E+00(2.03E-01) −	**1.3694E+00(2.14E-01)**
SMMOP2	3	100	1.3815E+01(8.11E+00) −	**1.5986E+00(2.71E-01)** +	1.1460E+01(1.53E+00) −	6.6176E+00(1.75E-01) −	7.2718E+00(4.01E-01) −	2.6709E+00(1.23E-01)
SMMOP3	3	100	1.3190E+01(1.28E+00) −	**8.2659E-01(5.89E-02)** +	1.1203E+01(8.20E+00) −	6.7243E+00(4.03E-01) −	8.2614E+00(5.68E-01) −	3.6382E+00(7.01E-01)
SMMOP4	3	100	1.3154E+01(3.20E+00) −	1.9553E+00(4.82E-01) −	9.1148E+00(6.49E-01) −	1.2327E+01(3.22E+00) −	6.9037E+00(1.91E-01) −	**1.5687E+00(8.24E-01)**
SMMOP5	3	100	1.2806E+01(1.80E+00) −	2.5320E+00(6.15E-01) −	7.6278E+00(6.03E-01) −	7.8509E+00(5.23E-01) −	5.5422E+00(7.40E-01) −	**2.1456E+00(2.37E-01)**
SMMOP6	3	100	1.3012E+01(7.14E+00) −	2.2557E+00(8.64E-01) −	**3.4919E-01**(1.63E-02) +	1.2077E+01(6.02E+00) −	7.9918E+00(5.22E-01) −	1.6419E+00(2.82E-01)
SMMOP7	3	100	1.2488E+01(9.30E+00) −	**1.0361E+00(9.65E-01)** +	4.3657E+00(2.46E-01) −	4.0809E+00(1.52E-01) −	4.1416E+00(3.74E-01) −	1.6286E+00(3.36E-01)
SMMOP8	3	100	1.2251E+01(8.91E+00) −	2.0442E+00(3.91E-01) −	4.5002E+00(1.52E-01) −	3.9522E+00(5.70E-01) −	4.0853E+00(2.16E-01) −	**1.9065E+00(1.96E-01)**
+/−/≈			0 / 20 / 0	5 / 14 / 1	4 / 16 / 0	2 / 17 / 1	3 / 16 / 1	/
RankSum			6.0000	2.8500	4.0000	2.9500	3.4000	1.8000

TABLE S-IV
1/PSP VALUES OF THREE ALGORITHMS ON MMMOPS AND SMMOPS, WHERE BEST RESULTS ON EACH TEST INSTANCE ARE IN BOLD

Problem	*D*	HREA	HHC-MMEA	CoMMEA	CMMO	MMEAPSL	NAIMEO(ours)
MMMOP1	10	1.1644E+00(4.05E-01) −	9.4187E-01(6.43E-02) −	8.0510E-01(6.13E-02) −	5.4686E-01(4.23E-02) −	7.8051E-01(3.16E-02) −	**4.3884E-01(1.54E-02)**
	10	1.0506E+00(3.22E-01) −	1.0285E+00(8.49E-01) −	8.1988E-01(5.18E-02) −	4.9072E-01(7.12E-02) −	6.0373E-01(4.27E-02) −	**4.8397E-01(4.81E-02)**
MMMOP2	10	1.0910E+00(5.01E-01) −	2.9321E-01(2.87E-02) −	1.4635E-01(3.76E-02) +	**1.0841E-01(9.51E-02)** +	1.2867E-01(9.57E-02) +	2.3565E-01(5.04E-02)
	10	1.0387E+00(7.31E-01) −	3.7132E-01(4.83E-02) +	9.3735E-01(5.18E-02) −	3.5628E-01(4.26E-02) +	4.5368E-01(2.46E-02) −	**2.9684E-01(6.18E-02)**
MMMOP3	10	9.6328E-01(8.76E-02) −	3.2313E-01(4.59E-02) −	2.7350E-01(4.33E-02) −	1.5766E-01(1.51E-02) −	**1.2346E-01(4.55E-02)** +	1.3845E-01(2.49E-02)
	10	1.1084E+00(2.50E-01) −	7.5366E-01(8.76E-02) −	8.3810E-01(1.03E-02) −	4.9020E-01(3.12E-02) −	5.6311E-01(7.26E-02) −	**4.2632E-01(2.65E-02)**
MMMOP4	10	1.1492E+00(3.48E-01) −	7.3965E-01(8.53E-02) −	7.0108E-01(1.56E-02) −	7.3284E-01(9.31E-02) −	8.4422E-01(6.57E-02) −	**4.0903E-01(2.25E-02)**
	10	1.1461E+00(2.74E-01) −	9.4813E-01(6.18E-02) −	1.0781E+00(4.02E-01) −	6.6599E-01(1.99E-02) −	7.7025E-01(2.05E-02) −	**4.3699E-01(6.87E-02)**
MMMOP5	10	1.1924E+00(6.27E-01) −	4.6491E-01(5.97E-02) +	7.9849E-01(5.27E-02) −	5.7213E-01(1.27E-02) −	7.3589E-01(8.17E-02) −	**4.5778E-01(9.39E-02)**
	10	1.2051E+00(2.55E-01) −	9.8715E-01(3.60E-02) −	1.1598E+00(7.92E-01) −	5.9007E-01(3.97E-02) −	7.9260E-01(8.43E-02) −	**4.3786E-01(4.02E-02)**
MMMOP6	10	3.0481E+00(6.59E-01) −	1.3346E+00(3.48E-01) +	**1.1687E+00(7.03E-01)** +	1.6572E+00(3.32E-01) ≈	3.0826E+00(4.65E-01) −	1.6437E+00(7.53E-01)
	10	1.6853E+00(3.49E-01) +	3.4646E+00(4.62E-01) −	**7.1184E-01(5.46E-02)** +	7.3300E-01(4.85E-02) +	8.2982E-01(1.16E-02) +	2.4405E+00(5.21E-01)
SMMOP1	100	1.3025E+01(6.92E+00) −	/	4.5737E+00(6.58E-01) −	4.6234E+00(4.58E-01) −	4.4535E+00(2.16E-01) −	**1.3694E+00(2.14E-01)**
SMMOP2	100	1.4017E+01(1.72E+00) −	/	1.1356E+01(5.17E+00) −	6.7910E+00(1.28E-01) −	7.2759E+00(3.04E-01) −	**2.6709E+00(1.23E-01)**
SMMOP3	100	1.3701E+01(2.62E+00) −	/	1.1379E+01(9.32E+00) −	7.4511E+00(2.20E-01) −	8.2741E+00(4.68E-01) −	**2.1640E+00(3.58E-01)**
SMMOP4	100	1.2943E+01(6.05E+00) −	2.3029E+00(4.57E-01) −	9.3793E+00(8.20E-01) −	1.2624E+01(5.44E+00) −	6.9648E+00(5.12E-01) −	**1.5689E+00(2.10E-01)**
SMMOP5	100	1.3072E+01(4.05E+00) −	2.3219E+00(1.97E-01) −	7.4438E+00(9.14E-01) −	7.5414E+00(5.19E-01) −	5.5904E+00(3.37E-01) −	**2.1462E+00(5.02E-01)**
SMMOP6	100	1.3234E+01(2.85E+00) −	/	8.4187E+00(3.55E-01) −	1.2178E+01(2.88E+00) −	8.5370E+00(3.53E-01) −	1.6424E+00(9.83E-01)
SMMOP7	100	1.2767E+01(2.02E+00) −	**7.1016E-01(8.65E-02)** +	4.8748E+00(5.81E-01) −	5.3013E+00(5.28E-01) −	5.4713E+00(8.70E-01) −	1.6287E+00(2.15E-01)
SMMOP8	100	1.2526E+01(1.24E+00) −	/	5.1901E+00(4.28E-01) −	5.3765E+00(8.49E-01) −	4.9776E+00(3.10E-01) −	**1.9495E+00(7.47E-01)**
+/−/≈		1 / 19 / 0	4 / 16 / 0	3 / 17 / 0	3 / 16 / 1	3 / 17 / 0	/
RankSum		5.6000	4.2000	3.5500	2.9000	3.2000	1.5500

"/" means the infinite

TABLE S-V
IGD VALUES OF TWO ALGORITHMS ON SMMOPS WITH THREE OBJECTIVES, WHERE BEST RESULTS ON EACH TEST INSTANCE ARE IN BOLD

Problem	*np*	*D*	HHC-MMEA	NAIMEO (ours)
SMMOP1	4	500	5.3940E-02(7.71E-03) −	**2.1291E-02(3.34E-03)**
		1000	5.4521E-02(8.38E-03) −	**2.0982E-02(5.85E-03)**
	8	500	4.8640E-02(9.75E-03) −	**2.1282E-02(6.74E-03)**
		1000	5.8164E-02(6.39E-03) −	**2.0945E-02(8.03E-03)**
SMMOP2	4	500	4.5543E-02(3.93E-03) −	**2.1923E-02(9.81E-03)**
		1000	5.2385E-02(2.12E-03) −	**2.8270E-02(7.02E-03)**
	8	500	5.4952E-02(2.33E-03) −	**2.1933E-02(9.52E-03)**
		1000	4.7401E-02(1.67E-03) −	**2.7335E-02(3.27E-03)**
SMMOP3	4	500	5.8801E-02(2.35E-03) −	**2.1412E-02(4.64E-03)**
		1000	9.0437E-02(8.15E-03) −	**2.2203E-02(6.31E-03)**
	8	500	7.4907E-02(3.66E-03) −	**2.0985E-02(4.22E-03)**
		1000	9.5261E-02(4.62E-03) −	**2.2974E-02(4.93E-03)**
SMMOP4	4	500	5.6094E-02(1.25E-03) −	**1.4962E-02(8.50E-03)**
		1000	7.7751E-02(6.65E-03) −	**1.6054E-02(7.58E-03)**
	8	500	6.5297E-02(5.89E-03) −	**1.4946E-02(8.27E-02)**
		1000	1.3354E-01(2.59E-02) −	**1.6344E-02(8.42E-03)**
SMMOP5	4	500	6.0091E-02(5.39E-03) −	**1.4715E-02(2.80E-03)**
		1000	5.2553E-02(6.82E-03) −	**2.0025E-02(7.44E-03)**
	8	500	3.4493E-02(8.43E-03) −	**1.4572E-02(4.23E-03)**
		1000	1.7336E-01(3.45E-02) −	**2.1998E-02(7.01E-03)**
SMMOP6	4	500	7.9945E-02(3.15E-03) −	**1.4921E-02(3.06E-03)**
		1000	5.4232E-02(1.92E-03) −	**1.7414E-02(4.45E-03)**
	8	500	9.8230E-02(7.66E-03) −	**1.4828E-02(2.42E-03)**
		1000	1.8173E-01(1.65E-02) −	**1.7452E-02(7.45E-03)**
SMMOP7	4	500	6.9523E-02(9.42E-03) −	**2.6552E-02(8.63E-03)**
		1000	1.3264E-01(7.87E-02) −	**3.6662E-02(9.35E-03)**
	8	500	8.9445E-02(7.58E-03) −	**3.1069E-02(2.10E-03)**
		1000	1.3253E-01(2.67E-02) −	**4.2405E-02(8.69E-03)**
SMMOP8	4	500	8.2924E-02(7.31E-03) −	**2.6902E-02(3.58E-03)**
		1000	9.6652E-02(9.29E-03) −	**4.6723E-02(3.50E-03)**
	8	500	7.8311E-02(4.04E-03) −	**2.6809E-02(6.51E-03)**
		1000	9.9761E-02(2.84E-03) −	**4.7028E-02(7.17E-03)**
+/−/≈			0 / 32 / 0	

TABLE S-VI
IGDX VALUES OF TWO ALGORITHMS ON SMMOPS WITH THREE OBJECTIVES, WHERE BEST RESULTS ON EACH TEST INSTANCE ARE IN BOLD

Problem	*np*	*D*	HHC-MMEA	NAIMEO (ours)
SMMOP1	4	500	6.6994E+00(7.71E-01) −	**9.0383E-01(5.03E-01)**
		1000	7.0603E+00(4.89E-01) −	**2.5492E+00(9.43E-01)**
	8	500	3.8626E+00(9.21E-01) −	**1.1853E+00(4.73E-01)**
		1000	8.1897E+00(6.03E-01) −	**7.9879E+00(5.58E-01)**
SMMOP2	4	500	3.8512E+00(5.85E-01) −	**1.0292E+00(2.03E-01)**
		1000	6.8728E+00(1.41E-01) −	**5.9313E+00(1.84E-01)**
	8	500	3.2487E+00(5.94E-01) −	**8.1762E-01(7.11E-02)**
		1000	**6.4975E+00(1.67E-01)** +	1.1039E+01(5.77E+00)
SMMOP3	4	500	**3.3341E+00(7.53E-01)** +	5.1048E+00(5.03E-01)
		1000	**7.3903E+00(4.27E-01)** +	1.0957E+01(9.20E+00)
	8	500	**4.1776E+00(3.07E-01)** +	5.6829E+00(3.65E-01)
		1000	**7.5346E+00(2.35E-01)** +	1.0974E+01(6.58E+00)
SMMOP4	4	500	4.1878E+00(1.25E-01) −	**1.0779E+00(4.40E-01)**
		1000	7.1123E+00(1.93E-01) −	**2.4979E+00(1.52E-01)**
	8	500	4.6754E+00(1.55E-01) −	**1.2122E+00(2.42E-01)**
		1000	6.6968E+00(4.25E-01) −	**5.3895E+00(6.33E-01)**
SMMOP5	4	500	4.4509E+00(8.56E-01) −	**1.4600E+00(8.32E-01)**
		1000	1.0436E+01(9.05E+00) −	**3.1705E+00(5.65E-01)**
	8	500	5.3884E+00(1.37E-01) −	**1.5548E+00(8.73E-01)**
		1000	7.3168E+00(7.45E-01) −	**3.2071E+00(1.97E-01)**
SMMOP6	4	500	4.9257E+00(5.38E-01) −	**1.1281E+00(5.53E-01)**
		1000	9.9840E+00(6.93E-01) −	**1.6045E+00(4.77E-01)**
	8	500	5.1714E+00(6.49E-01) −	**1.6045E+00(5.29E-01)**
		1000	7.7284E+00(1.65E-01) −	**5.1011E+00(2.55E-01)**
SMMOP7	4	500	**3.1662E+00(3.70E-01)** +	7.9856E+00(3.31E-01)
		1000	**6.9337E+00(2.19E-01)** +	1.1322E+01(5.44E+00)
	8	500	3.3421E+00(3.23E-01) −	**1.8591E+00(1.30E-01)**
		1000	**6.7306E+00(4.15E-01)** +	1.1415E+01(9.66E+00)
SMMOP8	4	500	**4.6101E+00(6.28E-01)** +	7.9316E+00(5.82E-01)
		1000	**7.9736E+00(3.14E-01)** +	1.1348E+01(1.33E+00)
	8	500	**4.3401E+00(7.03E-01)** +	6.8711E+00(3.65E-01)
		1000	**8.2051E+00(2.25E-01)** +	1.1213E+01(7.72E+00)
+/−/≈			12 / 20 / 0	

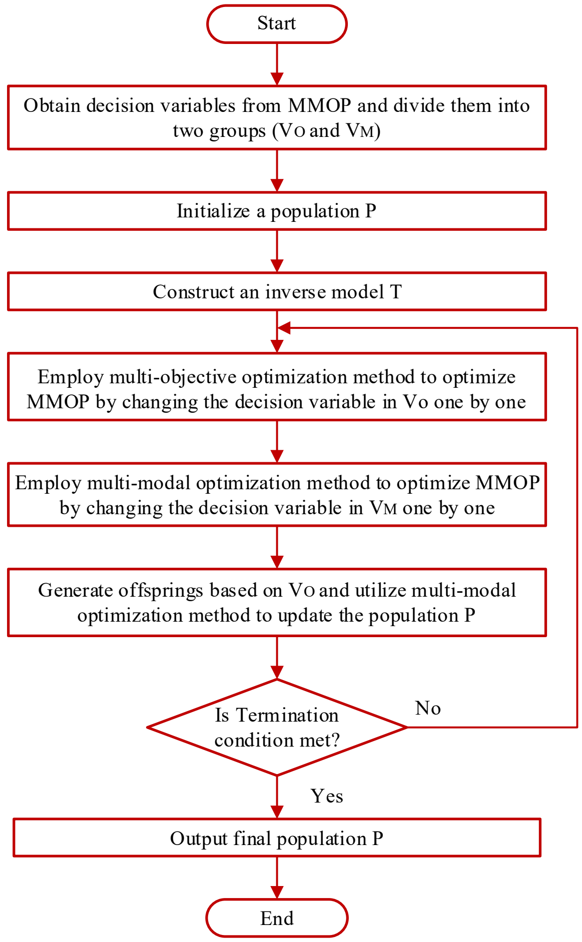

Fig. S-1. Framework of NAIMEO.

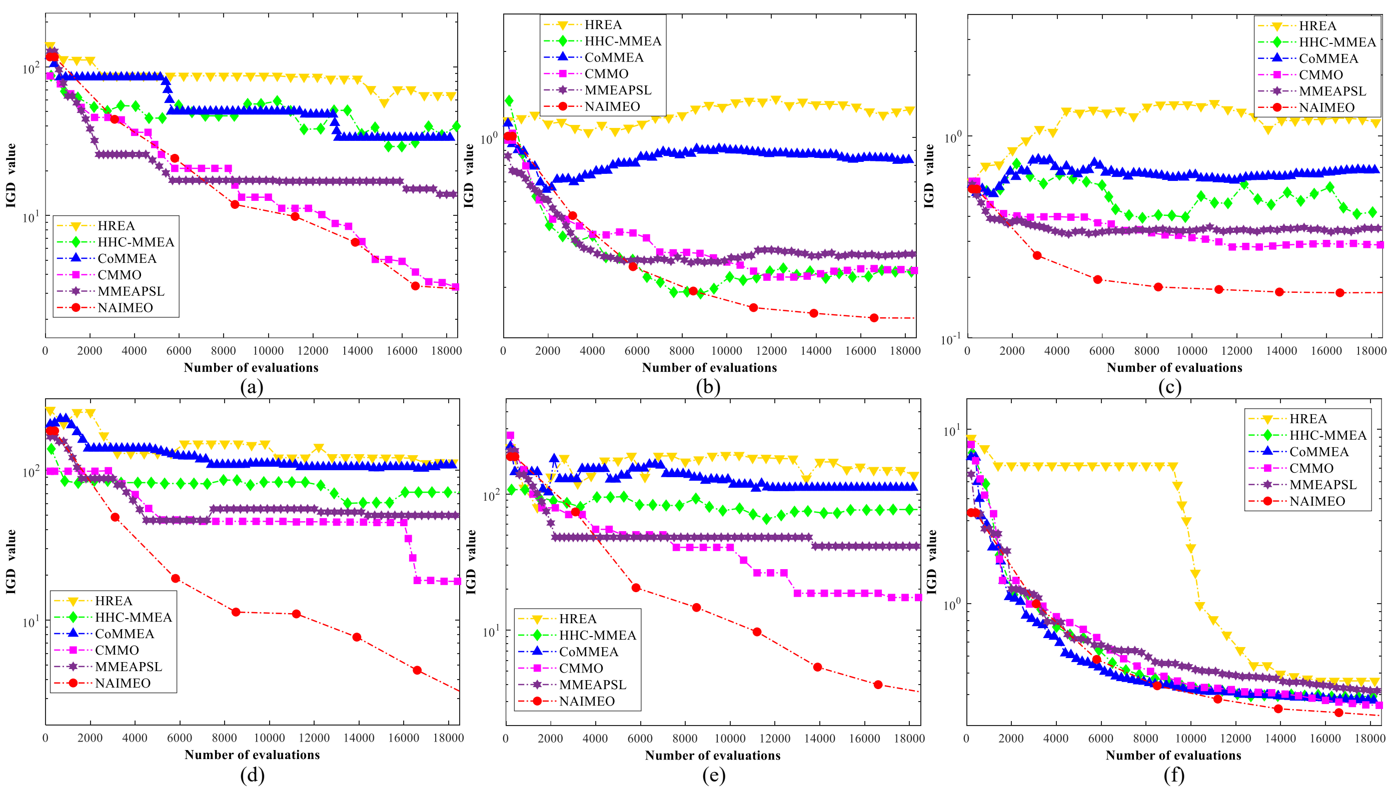

Fig. S-2. IGD values obtained by five algorithms on 5-objective 10-dimensional MMMOPs. (a)-(f) represent 5-objective MMMOP1-6.

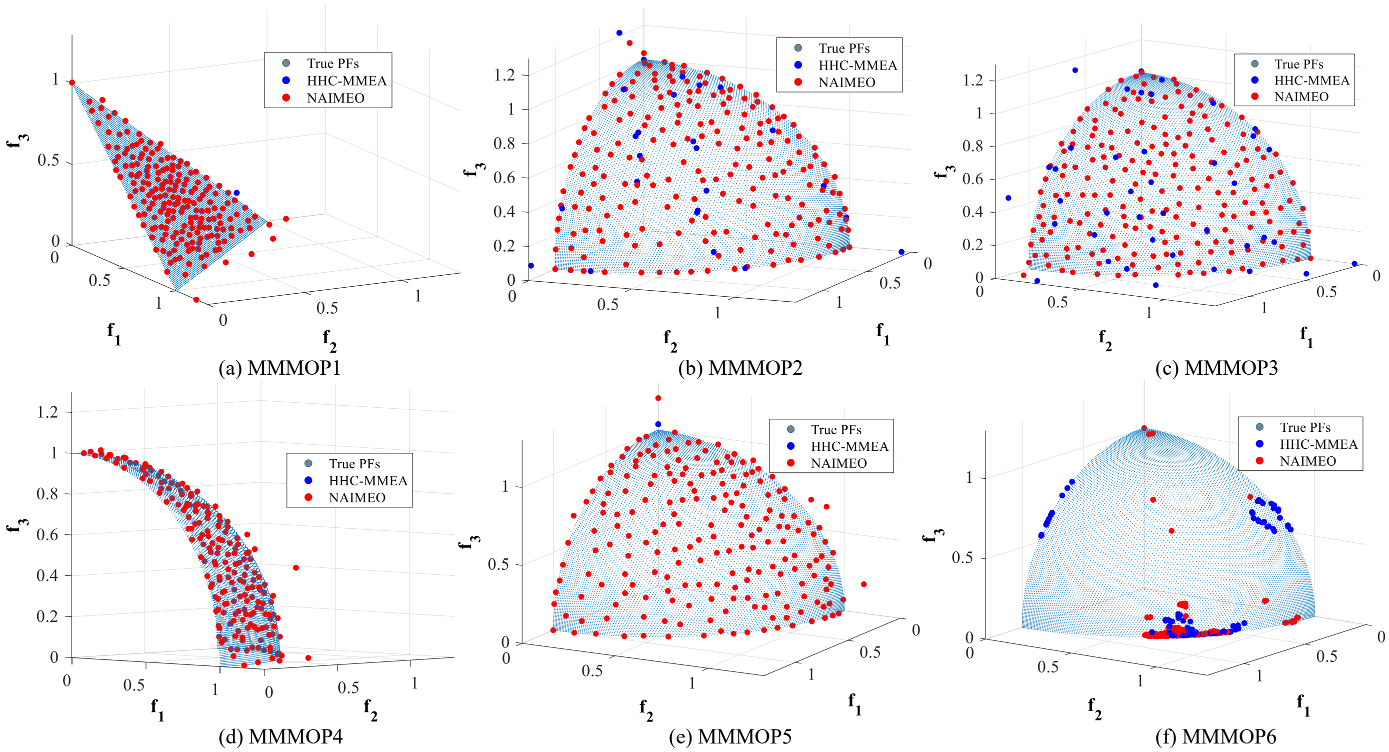

Fig. S-3. Distribution of two algorithms' results in objective spaces on MMMOP1-6 with 3 objectives and 10 decision variables. (a)-(f) represent MMMOP1-6.

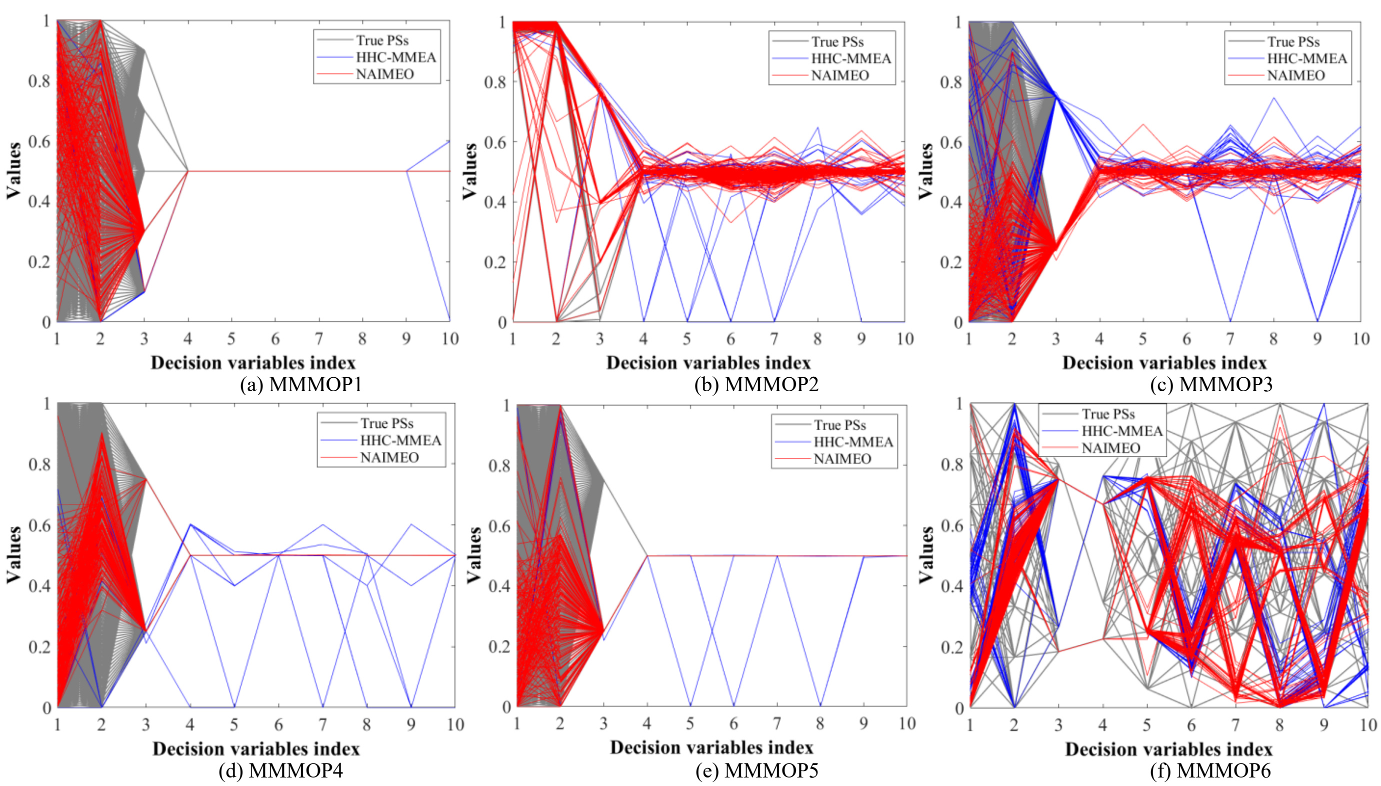

Fig. S-4. Distribution of two algorithms' results in decision spaces on MMMOP1-6 with 3 objectives and 10 decision variables. (a)-(f) represent MMMOP1-6.