SustainDC: Benchmarking for Sustainable Data Center Control
Supplementary Information

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Code, licenses, and setup instructions for SustainDC are available at GitHub[2]. The documentation can be accessed at [3].

A Models

A.1 Workload Environment (Env_{LS})

The Workload Environment (Env_{LS}) simulates the management and scheduling of data center (DC) workloads, allowing for dynamic adjustment of utilization to optimize energy consumption and carbon footprint. The environment is designed to evaluate the performance of reinforcement learning (RL) algorithms in rescheduling delay-capable workloads within the DC.

Let B_t be the instantaneous DC workload trace at time t, with $X\%$ of the load being rescheduled up to N simulation steps into the future. The goal of an RL agent ($Agent_{LS}$) is to observe the current time of day (SC_t), the current and forecast grid CI data ($CI_{t...t+L}$), and the amount of rescheduled workload left (D_t). Based on these observations, the agent decides an action $A_{ls,t}$ to reschedule the flexible component of B_t to create a modified workload $\hat{B}_t$, thus minimizing the net $CFP = \sum_{t=0}^{N} CFP_t$ over N steps. Here CFP_t will be calculated based on the sum of the DC IT load due to $\hat{B}_t$, the corresponding HVAC cooling load, and the charging and discharging of the battery at every time step.

A.1.1 Actions (A_{LS})

The action space for $Agent_{LS}$ includes three discrete actions:

- *Action 0: Decrease Utilization* - This action attempts to defer the flexible portion of the current workload ($B_{nonflex}$) to a later time. The non-flexible (B_{flex}) workload is processed immediately, while the flexible workload is added to a queue for future execution.
- *Action 1: Do Nothing* - This action processes both the flexible (B_{flex}) and non-flexible ($B_{nonflex}$) portions of the current workload immediately, without any deferral.
- *Action 2: Increase Utilization* - This action attempts to increase the current utilization by processing tasks from the queue, if available, in addition to the current workload.

A.1.2 Observations (S_{LS})

The state space observed by the RL agent consists of several features, including:

[2]GitHub repository: https://github.com/HewlettPackard/dc-rl.

[3]Documentation: https://hewlettpackard.github.io/dc-rl.

- **Time of Day** - Represented using sine and cosine transformations of the hour of the day to capture cyclical patterns.
- **Day of the Year** - Represented using sine and cosine transformations to capture seasonal variations.
- **Current Workload** - The current workload level, which includes both flexible and non-flexible components.
- **Queue Status** - The length of the task queue, normalized by the maximum queue length.
- **Grid Carbon Intensity (CI)** - Current and forecasted CI values, capturing the environmental impact of electricity consumption.
- **Battery State of Charge (SoC)** - The current state of charge of the battery, if available.

The observation space is a combination of these features, providing the agent with a comprehensive view of the current state of the environment.

A.1.3 Mathematical Model

Workload Breakdown Let B_t be the total workload at time t. This workload is divided into flexible ($B_{flex,t}$) and non-flexible ($B_{nonflex,t}$) components:

$$B_t = B_{flex,t} + B_{nonflex,t}$$

The flexible workload $B_{flex,t}$ is a fraction of the total workload:

$$B_{flex,t} = \alpha \cdot B_t, \quad 0 < \alpha < 1$$

where α is the flexible workload ratio.

Actions and Workload Management Depending on the action $A_{ls,t}$ chosen by the RL agent, the workload is managed as follows:

1. *Action 0: Decrease Utilization (Queue Flexible Workload)*

$$\hat{B}_t = B_{nonflex,t}$$

The flexible workload $B_{flex,t}$ is added to a task queue Q_t for future execution:

$$Q_{t+1} = Q_t + B_{flex,t}$$

2. *Action 1: Do Nothing*

$$\hat{B}_t = B_t = B_{nonflex,t} + B_{flex,t}$$

There is no change in the task queue:

$$Q_{t+1} = Q_t$$

3. *Action 2: Increase Utilization (Process Queue)*

$$\hat{B}_t = B_t + \min(Q_t, C_{max} - B_t)$$

where C_{max} is the maximum processing capacity. The processed tasks are removed from the task queue:

$$Q_{t+1} = Q_t - \min(Q_t, C_{max} - B_t)$$

A.2 Data Center Environment (Env_{DC})

The Data Center Environment (Env_{DC}) simulates the IT and HVAC operations within a DC, enabling the evaluation of RL algorithms aimed at optimizing cooling setpoints to reduce energy consumption and carbon footprint.

The data center modeled is illustrated in Figure 1. The IT section includes the cabinets and servers, while the Cooling section comprises a Cooling Tower, a chiller, and the Computer Room Air Handler (CRAH). The setup also features a raised floor system that channels cool air from the CRAH to the cabinets. The hot air exits the cabinets and returns to the CRAH via the ceiling.

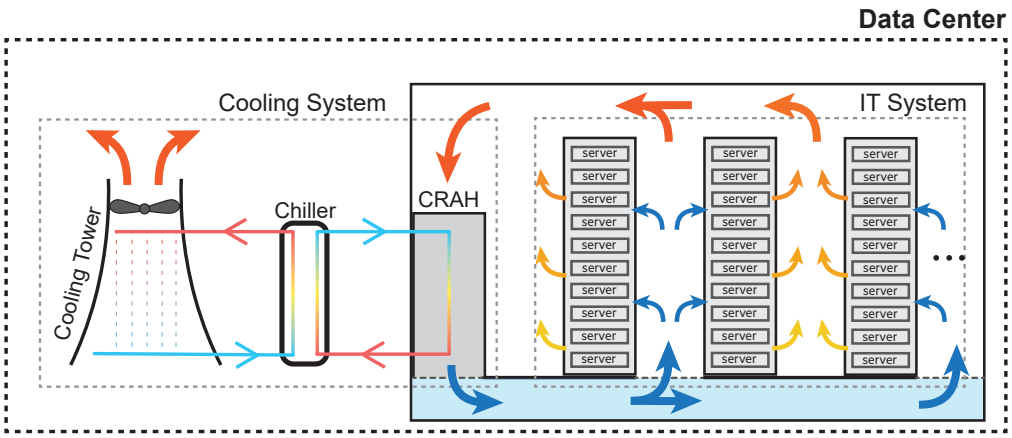

Figure 1: Illustration of the modeled data center, showing the IT section (cabinets and servers) and the Cooling section (Cooling Tower, chiller, and CRAH). The airflow path is also depicted, with cool air supplied through the raised floor and hot air returning via the ceiling. Note: We use CRAH and CRAC interchangeably in the text, but they both represent the same device (CRAH).

A.2.1 Data Center IT Model

Let $\hat{B}_t$ be the net DC workload at time instant t obtained from the Workload Manager. The spatial temperature difference, $\mathbf{\Delta T}_{supply}$, given the DC configuration, is obtained from Computational Fluid Dynamics (CFD). For a given rack, the inlet temperature $T_{inlet,i}$ at CPU_i is computed as:

$$T_{inlet,i,t} = \mathbf{\Delta T}_{supply,i} + T_{CRACsupply,t}$$

where $T_{CRACsupply,t}$ is the CRAC unit supply air temperature. This value is chosen by the RL agent A_{DC}.

Next, the CPU power curve $f_{cpu}(inlet\_temp, cpu\_load)$ and IT Fan power curve $f_{itfan}(inlet\_temp, cpu\_load)$ are implemented as linear equations based on (1). Given a server inlet temperature of $T_{inlet,i,t}$ and a processing amount of $\hat{B}_t$ performed by CPU_i, the total rack power consumption for rack k across all CPUs from $i = 1$ to K, and the total DC Power IT Consumption can be calculated as follows:

$$P_{CPU,t} = \sum_i f_{cpu}(T_{inlet,i,t}, \tilde{B}_t)$$

$$P_{IT\ Fan,t} = \sum_i f_{itfan}(T_{inlet,i,t}, \tilde{B}_t)$$

$$P_{rack,k,t} = P_{CPU,t} + P_{IT\ Fan,t}$$

$$P_{datacenter,t} = \sum_k P_{rack,k,t}$$

A.2.2 HVAC Cooling Model

Based on the DC IT Load $P_{datacenter,t}$, the IT fan airflow rate, V_{sfan}, air thermal capacity C_{air}, and air density, ρ_{air}, the rack outlet temperature $T_{outlet,i,t}$ is estimated from (1) using:

$$T_{outlet,i,t} = T_{inlet,i,t} + \frac{P_{rack,k,t}}{C_{air} \cdot \rho_{air} \cdot V_{sfan}}$$

In conjunction with the return temperature gradient information $\mathbf{\Delta T}_{return}$ estimated from CFDs, the final CRAC return temperature is obtained as:

$$T_{CRACreturn,t} = \text{avg}(\mathbf{\Delta T}_{return,i} + T_{outlet,i,t})$$

We assume a fixed-speed CRAC Fan unit for circulating air through the IT Room. Hence, the total HVAC cooling load for a given CRAC setpoint $T_{CRACsupply,t}$, return temperature $T_{CRACreturn,t}$,

and the mass flow rate $m_{crac,fan}$ is calculated as:

$$P_{cool,t} = m_{crac,fan} \cdot C_{air} \cdot (T_{CRACreturn,t} - T_{CRACsupply,t})$$

To perform $P_{cool,t}$, the amount of cooling, the net chiller load for a chiller with Coefficient of Performance (COP) may be estimated as:

$$P_{chiller,t} = P_{cool,t} \left(1 + \frac{1}{COP}\right)$$

Next, this cooling load is passed on to the cooling tower. Assuming a cooling tower delta as a function of temperature $f_{ct\_delta}(t_{db})$, (2) the required cooling tower air flow rate is calculated as:

$$V_{ct,air,t} = \frac{P_{chiller,t}}{C_{air} \cdot \rho_{air} \cdot f_{ct\_delta}(t_{db})}$$

Finally, the Cooling Tower Load at a flow rate of $V_{ct,air,t}$ is calculated with respect to a reference air flow rate $V_{ct,air,REF}$ and power consumption $P_{ct,REF}$ from the configuration object:

$$P_{CT,t} = P_{ct,REF} \left(\frac{V_{ct,air,t}}{V_{ct,air,REF}}\right)^3$$

Thus, the total HVAC load includes the cooling tower and chiller loads:

$$P_{HVAC,t} = P_{CT,t} + P_{chiller,t}$$

Based on these power values, the IT and HVAC Cooling energy consumptions can be represented as:

$$E_{hvac,t} = P_{HVAC,t} \times \text{step size} \quad (1)$$

$$E_{it,t} = P_{datacenter,t} \times \text{step size} \quad (2)$$

A.2.3 Actions (A_{DC})

The action space for $Agent_{DC}$ consists of discrete actions representing the adjustment of the CRAC unit's supply air temperature, limited to a range between 16°C to 23°C:

- *Action 0: Decrease Temperature* - The agent decreases the CRAC supply air temperature, enhancing cooling performance but increasing energy consumption.
- *Action 1: Maintain Temperature* - The agent maintains the current CRAC supply air temperature.
- *Action 2: Increase Temperature* - The agent increases the CRAC supply air temperature, which can reduce cooling energy consumption but may increase the IT equipment temperature.

A.2.4 Observations (S_{DC})

The state space observed by the RL agent consists of several features, including:

- **Time of Day** - Represented using sine and cosine transformations of the hour of the day to capture cyclical patterns.
- **Day of the Year** - Represented using sine and cosine transformations to capture seasonal variations.
- **Ambient Weather** - Includes current temperature and other relevant weather conditions.
- **IT Room Temperature** - Average temperature in the IT room.
- **Energy Consumption** - Previous step cooling and IT energy consumptions.
- **Grid Carbon Intensity (CI)** - Current and forecasted CI values.

The observation space provides a comprehensive view of the current state of the environment to the agent.

A.2.5 Chiller Sizing

The chiller power consumption is calculated based on the load and operating conditions using the following method:

$$P_{chiller,t} = \text{calculate\_chiller\_power}(max\_cooling\_cap, load, ambient\_temp)$$

Calculation of Average CRAC Return Temperature

$$T_{CRACreturn,t} = \text{avg}(\mathbf{\Delta T}_{return,i} + T_{outlet,i,t})$$

Calculation of HVAC Power

$$P_{cool,t} = m_{crac,fan} \cdot C_{air} \cdot (T_{CRACreturn,t} - T_{CRACsupply,t})$$

$$P_{chiller,t} = P_{cool,t} \left(1 + \frac{1}{COP}\right)$$

$$V_{ct,air,t} = \frac{P_{chiller,t}}{C_{air} \cdot \rho_{air} \cdot f_{ct\_delta}(t_{db})}$$

$$P_{CT,t} = P_{ct,REF} \left(\frac{V_{ct,air,t}}{V_{ct,air,REF}}\right)^3$$

$$P_{HVAC,t} = P_{CT,t} + P_{chiller,t}$$

A.2.6 Water Consumption Model

The water usage for the cooling tower is estimated using a model based on research findings from several key sources. The model accounts for the water loss due to evaporation, drift, and blowdown. The primary references used to develop this model include (3), (4), and guidelines from SPX Cooling Technologies (5).

The water usage model is formulated as follows:

1. **Range Temperature Calculation**: The difference between the hot water temperature entering the cooling tower and the cold water temperature leaving the cooling tower:

$$\text{range\_temp} = \text{hot\_water\_temp} - \text{cold\_water\_temp}$$

where hot_water_temp is the $T_{CRACreturn,t}$, and cold_water_temp is the current CRAC setpoint $T_{CRACsupply,t}$.

2. **Normalized Water Usage**: The baseline water usage per unit time, adjusted for the wet bulb temperature of the ambient air. This accounts for the environmental conditions affecting the cooling tower's efficiency:

$$\text{norm\_water\_usage} = 0.044 \cdot \text{wet\_bulb\_temp} + (0.35 \cdot \text{range\_temp} + 0.1)$$

3. **Total Water Usage**: The normalized water usage is adjusted to ensure non-negativity and further adjusted for drift losses, which are a small percentage of the total water circulated in the cooling tower:

$$\text{water\_usage} = \max(0, \text{norm\_water\_usage}) + \text{norm\_water\_usage} \cdot \text{drift\_rate}$$

4. **Water Usage Conversion**: The total water usage is converted to liters per simulation timestep interval for ease of reporting and consistency with other metrics. Given that we use N timesteps per hour in our simulations, the conversion is as follows:

$$\text{water\_usage\_liters\_per\_timestep} = \left(\frac{\text{water\_usage} \cdot 1000}{N}\right)$$

This model incorporates both theoretical and empirical insights, providing a comprehensive estimation of the water consumption in a data center's cooling tower. By considering the specific operational parameters and environmental conditions, it ensures accurate and reliable water usage calculations, critical for sustainable data center management.

A.3 Battery Environment (Env_{BAT})

The Battery Environment (Env_{Bat}) simulates the battery banks operations within the DC, enabling the evaluation of RL algorithms aimed at optimizing auxiliary battery usage to reduce energy costs and carbon footprint. This environment is a modified version of the battery model from (6).

A.3.1 Battery Model

The battery model represents the energy storage system, considering its capacity, charging and discharging efficiency, and rate limits. The battery state of charge (SoC) evolves based on the actions taken by the RL agent.

Let $E_{bat,t}$ be the energy stored in the battery at time t. The battery can perform three actions: charge, discharge, or remain idle. The maximum battery capacity is C_{max}, and the current state of charge is $E_{bat,t}$.

A.3.2 Actions (A_{Bat})

The action space for $Agent_{Bat}$ includes three discrete actions:

- *Action 0: Charge* - The battery is charged at a rate of r_{charge}, consuming $E_{bat,t}$ Wh of energy.
- *Action 1: Idle* - The battery do not consume energy.
- *Action 2: Discharge* - The battery discharges energy at a rate of $r_{discharge}$, supplying $E_{bat,t}$ Wh of energy.

A.3.3 Observations (S_{Bat})

The state space observed by the RL agent consists of several features, including:

- **Data Center Load** - The current power consumption of the data center.
- **Battery SoC** - The current state of charge of the battery.
- **Grid Carbon Intensity (CI)** - Current and forecasted CI values.
- **Time of Day and Year** - Represented using sine and cosine transformations to capture cyclical patterns.

The observation space is a combination of these features, providing the agent with a comprehensive view of the current state of the environment.

A.3.4 Mathematical Model

Battery Charging and Discharging The energy stored in the battery evolves based on the action taken:

$$E_{bat,t} = \begin{cases} r_{charge} \cdot \eta_{charge} \cdot \Delta t & \text{if charging} \\ 0 & \text{if idle} \\ r_{discharge} \cdot \eta_{discharge} \cdot \Delta t & \text{if discharging} \end{cases}$$

where r_{charge} and $r_{discharge}$ are the rates of charging and discharging the battery, respectively. These rates determine the amount of energy added to or removed from the battery within a time step Δt.

Charging Rate (r_{charge}) The charging rate r_{charge} is the rate at which energy is added to the battery during the charging process. It is defined as:

$$r_{charge} = \min\left(\frac{C_{max} - E_{bat,t}}{\eta_{charge} \cdot \Delta t}, P_{charge,max}\right)$$

where $P_{charge,max}$ is the maximum allowable charging power. This rate ensures that the battery does not exceed its maximum capacity C_{max} and that charging occurs efficiently.

Discharging Rate ($r_{discharge}$) The discharging rate $r_{discharge}$ is the rate at which energy is drawn from the battery during the discharging process. It is defined as:

$$r_{discharge} = \min\left(\frac{E_{bat,t}}{\eta_{discharge} \cdot \Delta t}, P_{discharge,max}\right)$$

where $P_{discharge,max}$ is the maximum allowable discharging power. This rate ensures that the battery does not discharge below zero and that discharging occurs efficiently.

Energy Constraints The state of charge is bounded by the battery capacity:

$$0 \leq E_{bat,t} \leq C_{max}$$

Battery Power Constraints The maximum power that the battery can charge or discharge is limited by:

$$P_{charge,max} = u \cdot P_{charge} + v$$
$$P_{discharge,max} = u \cdot P_{discharge} + v$$

Simple Reward Calculation The goal of the three agents ($Agent_{LS}$, $Agent_{DC}$, and $Agent_{BAT}$) is to minimize the cumulative carbon footprint (CFP) over a given horizon N. The CFP at each time step t is computed as:

$$CFP_t = (E_{it,t} + E_{hvac,t} + E_{bat,t}) \cdot CI_t$$

where:

- $E_{it,t}$: Energy consumption by IT equipment due to $\hat{B}_t$
- $E_{hvac,t}$: Energy consumption by HVAC systems
- $E_{bat,t}$: Energy contribution from the battery (positive when discharging, negative when charging)
- CI_t: Grid carbon intensity at time t

The total reward is then:

$$R = -\sum_{t=0}^{N} CFP_t$$

The reward could have other terms that may consider queue length, water usage, average task delay, etc.

A.4 Interconnection of Environments and Agent Actions

Figure 2 illustrates the interconnection of the different environments (Env_{LS}, Env_{DC}, and Env_{BAT}) and the actions of their respective RL agents. This diagram highlights how the decisions made by each agent impact the overall DC operations and contribute to the optimization of energy consumption and carbon footprint.

In the **Workload Environment** (Env_{LS}), the RL agent ($Agent_{LS}$) reschedules flexible workloads to optimize utilization. This action will influence the IT load, which directly impacts the **Data Center Environment** (Env_{DC}). The RL agent ($Agent_{DC}$) in the data center environment adjusts the CRAC setpoints to optimize cooling and IT operations, thus affecting the HVAC cooling load and overall energy consumption.

The **Battery Environment** (Env_{BAT}) is influenced by the energy demands of the data center environment. The RL agent ($Agent_{BAT}$) manages the charging and discharging of the battery to optimize energy usage and reduce the carbon footprint. The interconnections between these environments ensure that the agents work together to minimize the cumulative CFP by considering the energy consumption of IT, HVAC, and battery systems.

By observing the current state and forecast data, each agent makes informed decisions that contribute to the overall sustainability and efficiency of the data center operations. This coordinated approach leverages the strengths of each environment to achieve significant reductions in energy consumption and carbon emissions.

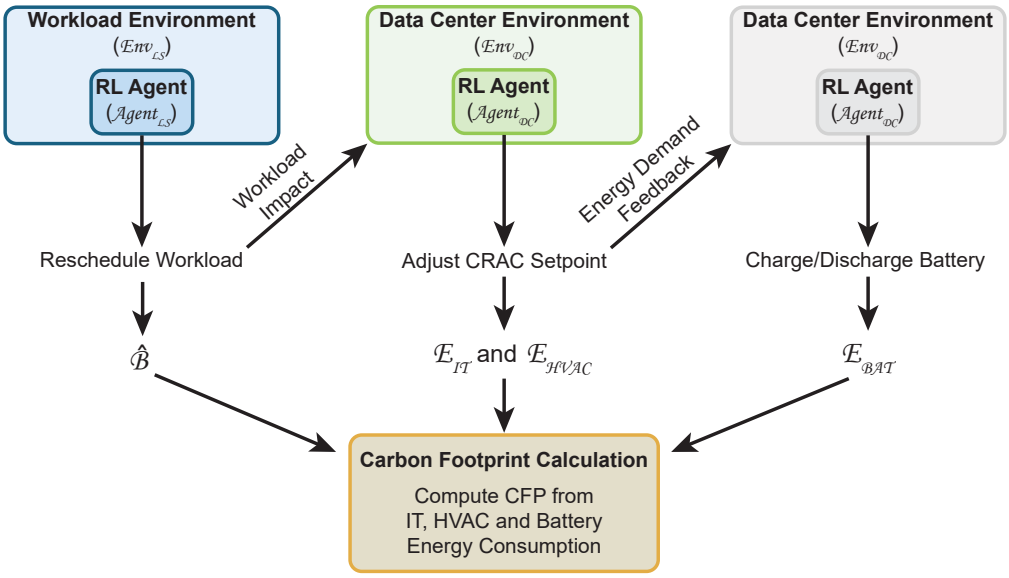

Figure 2: Interconnection of environments and agent actions. The figure shows how the Workload Environment (Env_{LS}) interacts with the Data Center Environment (Env_{DC}) by rescheduling workloads, and how the Data Center Environment impacts the Battery Environment (Env_{BAT}) through energy demands. Each agent observes the state of its respective environment and takes actions to optimize operations, with the overall goal of minimizing the carbon footprint (CFP) through coordinated efforts.

B Customization of *dc_config.json*

The customization of the DC is done through the `dc_config.json` file located in the utils folder. This file allows users to specify every aspect of the DC environment design. We show here a part of the configuration file to indicate the different configurable elements inside SustainDC. Additional elements can be added to this config either under an existing section or a new section, and `utils/dc_config_reader.py` will automatically import the new configurations. Inside the "`data_center_configuration`" SustainDC allows the user to configure the dimensions of the data center arrangement, the compiled CFD supply and approach temperature delta values and the maximum allowable CPUs per rack. There is an extensive set of parameters that can be configured under the "`hvac_configuration`" section including physical constants, parameters of the computer room air-conditioning unit (CRAC), chiller, pumps and cooling towers. The "`server_characteristics`" block allows the user to specify the properties of individual servers in the data center, including their idle power, full load fan frequency and power.

```
{
"data_center_configuration" :
{
    "NUM_ROWS" : 4,
    "NUM_RACKS_PER_ROW" : 5,
    "RACK_SUPPLY_APPROACH_TEMP_LIST" : [
                                        5.3, 5.3, 5.3, 5.3,5.3,
                                        5.0, 5.0, 5.0, 5.0,5.0,
                                        5.0, 5.0, 5.0, 5.0,5.0,
                                        5.3, 5.3, 5.3, 5.3, 5.3
                                        ],
    "RACK_RETURN_APPROACH_TEMP_LIST" :  [
                                        -3.7, -3.7, -3.7, -3.7, -3.7,
                                        -2.5, -2.5, -2.5, -2.5, -2.5,
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                                        -3.7, -3.7, -3.7, -3.7, -3.7
                                        ],
    "CPUS_PER_RACK" : 200
},
"hvac_configuration" :
{
    "C_AIR" : 1006,
```

```
        "RHO_AIR" : 1.225,
        "CRAC_SUPPLY_AIR_FLOW_RATE_pu" : 0.00005663,
        "CRAC_REFRENCE_AIR_FLOW_RATE_pu" : 0.00009438,
        "CRAC_FAN_REF_P" : 150,
        "CHILLER_COP_BASE" : 5.0,
        "CHILLER_COP_K" : 0.1,
        "CHILLER_COP_T_NOMINAL" : 25.0,
        "CT_FAN_REF_P" : 1000,
        "CT_REFRENCE_AIR_FLOW_RATE" : 2.8315,
        "CW_PRESSURE_DROP" : 300000,
        "CW_WATER_FLOW_RATE" : 0.0011,
        "CW_PUMP_EFFICIENCY" : 0.87,
        "CT_PRESSURE_DROP" : 300000,
        "CT_WATER_FLOW_RATE" : 0.0011,
        "CT_PUMP_EFFICIENCY" : 0.87

    },
    "server_characteristics" :
    {
        "CPU_POWER_RATIO_LB" : [0.01, 1.00],
        "CPU_POWER_RATIO_UB" : [0.03, 1.02],
        "IT_FAN_AIRFLOW_RATIO_LB" : [0.01, 0.225],
        "IT_FAN_AIRFLOW_RATIO_UB" : [0.225, 1.0],
        "IT_FAN_FULL_LOAD_V" : 0.051,
        "ITFAN_REF_V_RATIO" : 1.0,
        "ITFAN_REF_P" : 10.0,
        "INLET_TEMP_RANGE" : [16, 28],
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        "HP_PROLIANT" : [110,170]
    }
}
```


C Performance of RL agents on Evaluation Metrics

In this section, we provide the numerical results we obtained from the main paper. The results are shown in Tables 1 (advantage of multiagent vs single agent), 2 (effects of reward sharing across agents), 3, 4, 5 and 6 (ablation across geographical locations with different weather, grid carbon intensity and server load pattern). We observed that there is not a single algorithm that works well across different metrics and geographical locations, and this is visually appreciated in the main paper.

Table 1: Performance with respect to evaluation metrics on single and multiple RL agent baselines. $A_* : RL\ agent\ B_* : non-RL\ baseline\ agent$

Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
1:$A_{LS} + B_{DC} + B_{BAT}$	167.61	391.6	1033.8	0.52	10433.46
2:$B_{LS} + A_{DC} + B_{BAT}$	153.56	372.9	944.5	0.0	10930.77
3:$B_{LS} + B_{DC} + A_{BAT}$	168.22	390.3	1029.8	0.0	10493.95
4: $A_{LS} + A_{DC} + B_{BAT}$	155.97	374.9	941.3	0.48	10883.73
5:$A_{LS} + B_{DC} + A_{BAT}$	168.64	391.1	1030.9	0.56	10470.43
6:$B_{LS} + A_{DC} + A_{BAT}$	155.44	374.8	942.5	0	10883.73
7:$A_{LS} + A_{DC} + A_{BAT}$	155.23	371.8	937.4	0.45	10826.61

Table 2: IPPO evaluated on SustainDC with different values of collaborative reward coefficient α (Average result over 12 runs)

Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
IPPO($\alpha = 1.0$)	176.3	415.2	932.8	12.5	445.6
IPPO($\alpha = 0.8$)	176.2	414.6	932.8	9.5	445.8
IPPO($\alpha = 0.1$)	176.4	415.3	932.9	15.7	446.2

Table 3: Multiagent RL framework evaluated on SustainDC for a data center located in New York (Average result over 5 runs)

Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
IPPO	179.6	417.1	945.9	20.9	446.2
MAPPO	176.4	417.0	932.7	19.6	446.2
HAPPO	177.3	414.8	930.9	12.8	441.9
HAA2C	177.5	419.0	934.8	25.2	14977.1
HAD3QN	178.4	420.5	940.4	28.0	14950.9
HASAC	181.7	424.2	960.8	79.7	14842.4

Table 4: Multiagent RL framework evaluated on SustainDC for a data center located in Georgia (Average result over 5 runs)

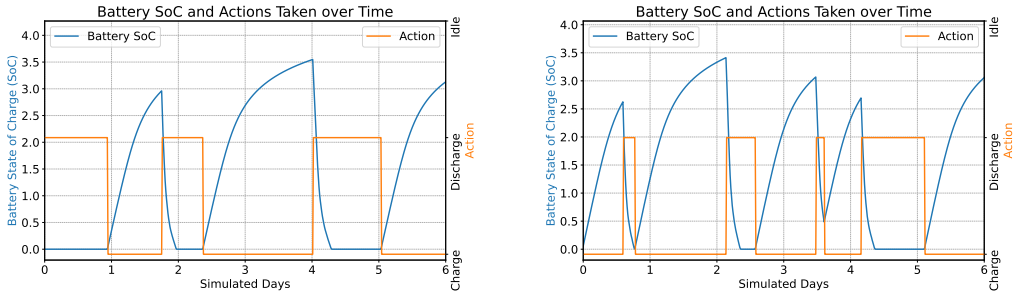
Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
IPPO	265.4	376.7	935.4	6.8	31773.5
MAPPO	263.4	370.3	935.9	0.35	31949.9
HAPPO	264.1	370.4	929.0	0.47	31890.7
HAA2C	262.7	367.1	928.3	6.6	32071.5
HAD3QN	262.8	370.7	935.1	0.0	31952.2
HASAC	263.0	367.4	932.4	0.0	32135.7

Table 5: Multiagent RL framework evaluated on SustainDC for a data center located in California (Average result over 5 runs)

Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
IPPO	170.0	384.3	933.8	12.9	28141.4
MAPPO	159.3	388.2	936.1	19.5	33289.3
HAPPO	159.1	376.3	935.8	74.9	30141.8
HAA2C	158.7	381.7	933.5	54.1	30135.4
HAD3QN	161.5	378.4	929.6	25.8	30017.4
HASAC	172.9	434.4	1027.0	43.8	29277.5

Table 6: Multiagent RL framework evaluated on SustainDC for a data center located in Arizona (Average result over 5 runs)

Evaluation Metric → Algorithm ↓	CFP (kgCO2)	HVAC Energy (kwh)	IT Energy (kwh)	Task Queue	Water Usage (litre)
IPPO	408.7	380.8	934.8	0.60	30251.6
MAPPO	410.8	383.3	947.5	502.4	31289.6
HAPPO	405.5	381.9	936.6	0.26	30983.7
HAA2C	407.1	385.0	929.9	7.54	32706.3
HAD3QN	405.6	386.4	1094.0	0.0051	30377.3
HASAC	404.6	380.8	936.7	0.54	30878.7



(a) Battery behavior example 1

(b) Battery behavior example 2

Figure 3: Battery State of Charge (SoC) and actions taken over time under two different random behaviors. The actions are labeled as Charge, Discharge, and Idle.

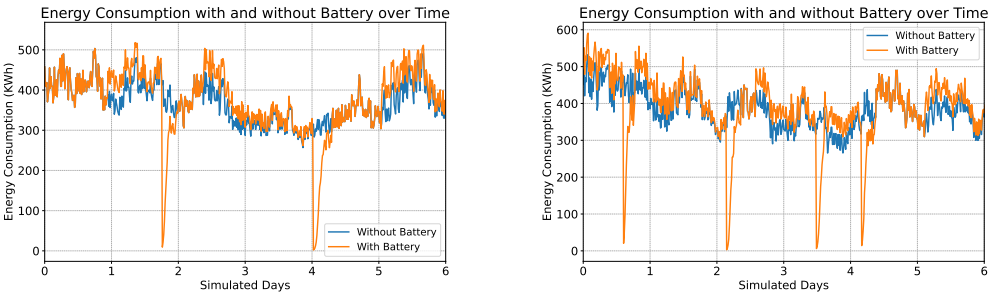
D Agents/Env behavior

D.1 Battery

The battery environment demonstrates how the battery's state of charge (SoC) and actions evolve over time under random behaviors. These figures illustrate two different examples generated using distinct random seeds.

Figure 3 shows the battery's SoC and the actions taken (Charge, Discharge, Idle) over simulated days for two different random behaviors.

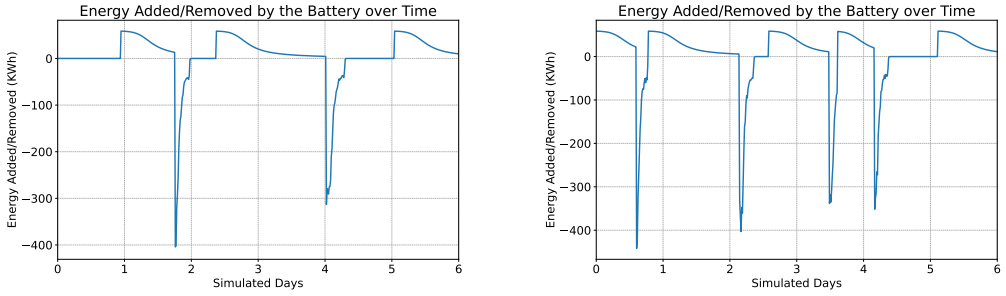
Figure 4 compares the energy consumption with and without the battery over simulated days for two different random behaviors. This comparison illustrates the impact of battery usage on the overall energy consumption of the data center.



(a) Battery behavior example 1

(b) Battery behavior example 2

Figure 4: Energy consumption with and without the battery over time under two different random behaviors. The comparison illustrates the effect of battery usage on overall energy consumption.



(a) Battery behavior example 1

(b) Battery behavior example 2

Figure 5: Energy added to and removed from the battery over time under two different random behaviors. The figures show how the battery charges and discharges energy throughout the simulated period.

Figure 5 shows the energy added to and removed from the battery over simulated days for two different random behaviors. These figures demonstrate how the battery charges and discharges energy, providing insights into its operational patterns.

E External variables

E.1 Workload

The *Workload* external variable in SustainDC represents the computational demand placed on the data center. Workload traces are provided in the form of FLOPs (floating-point operations) required by various jobs. By default, SustainDC includes a collection of open-source workload traces from *Alibaba* (7) and *Google* (8) data centers. Users can customize this component by adding new workload traces to the *data/Workload* folder or specifying a path to existing traces in the *sustaindc_env.py* file under the `workload_file` configuration. Below is an example of modifying the workload configuration:

```
class EnvConfig(dict):

    DEFAULT_CONFIG = {
        "workload_file": "data/Workload/Alibaba_CPU_Data_Hourly_1.csv",
        ...
    }
```

The workload file should contain one year of data with an hourly periodicity (365*24=8760 rows). The file structure should have two columns, where the first column does not have a name, and the second column should be named `cpu_load`. Below is an example of the file structure:

```
,cpu_load
1,0.380
2,0.434
3,0.402
4,0.485
...
```

Figure 6 shows examples of different workload traces from Alibaba (v2017) and Google (v2011) data centers. Figure 7 provides a comparison between two workload traces of Alibaba (v2017) and Google (v2011).

E.2 Weather

The *Weather* external variable in SustainDC captures the ambient environmental conditions impacting the data center's cooling requirements. By default, SustainDC includes weather data files in the .epw format from `https://energyplus.net/weather` for various locations where data centers are commonly situated. These locations include Arizona, California, Georgia, Illinois, New York, Texas, Virginia, and Washington. Users can customize this component by adding new weather files to the *data/Weather* folder or specifying a path to existing weather files in the *sustaindc_env.py* file under the `weather_file` configuration. Below is an example of modifying the weather configuration:

```
class EnvConfig(dict):

    DEFAULT_CONFIG = {
        'weather_file': 'data/Weather/USA_NY_New.York-Kennedy.epw',
        ...
    }
```

Each .epw file contains hourly data for various weather parameters, but for our purposes, we focus on the ambient temperature. Figure 8 shows the typical average ambient temperature across different locations over one year. Figure 9 provides a comparison of external temperatures across the different selected locations.

E.3 Carbon Intensity

The *Carbon Intensity (CI)* external variable in SustainDC represents the carbon emissions associated with electricity consumption. By default, SustainDC includes CI data files for various locations: Arizona, California, Georgia, Illinois, New York, Texas, Virginia, and Washington. These files are located in the *data/CarbonIntensity* folder and are extracted from `https://api.eia.gov/bulk/EBA.zip`. Users can customize this component by adding new CI files to the *data/CarbonIntensity* folder or specifying a path to existing files in the *sustaindc_env.py* file under the `cintensity_file` configuration. Below is an example of modifying the CI configuration:

```
class EnvConfig(dict):

    DEFAULT_CONFIG = {
        'cintensity_file': 'data/CarbonIntensity/NY_NG_&_avgCI.csv',
        ...
    }
```

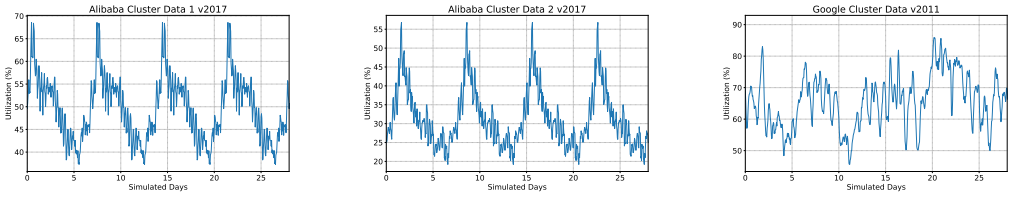
The CI file should contain one year of data with an hourly periodicity (365*24=8760 rows). The file structure should have the following columns: `timestamp`, `WND`, `SUN`, `WAT`, `OIL`, `NG`, `COL`, `NUC`, `OTH`, and `avg_CI`. `WND`, `SUN`, `WAT`, `OIL`, `NG`, `COL`, `NUC`, and `OTH` represent the energy sources contributing to the carbon intensity. These sources include wind, solar, water, oil, natural gas, coal, nuclear, and other types of energy, respectively. Below is an example of the file structure:

```
timestamp,WND,SUN,WAT,OIL,NG,COL,NUC,OTH,avg_CI
2022-01-01 00:00:00+00:00,1251,0,3209,0,15117,2365,4992,337,367.450
2022-01-01 01:00:00+00:00,1270,0,3022,0,15035,2013,4993,311,363.434
2022-01-01 02:00:00+00:00,1315,0,2636,0,14304,2129,4990,312,367.225
2022-01-01 03:00:00+00:00,1349,0,2325,0,13840,2334,4986,320,373.228
...
```

In Figure 10, the average daily carbon intensity for each selected location is shown, highlighting the variations in carbon emissions associated with electricity consumption across different regions.

In Figure 11, a comparison of carbon intensity across all the selected locations is presented, providing a comprehensive overview of how carbon emissions vary between these areas.

In Figure 12, we show the average daily carbon intensity against the average daily coefficient of variation (CV) for various locations. This figure highlights an important perspective on the variability and magnitude of carbon intensity values across different regions. Locations with a high CV indicate greater fluctuation in carbon intensity, offering more "room to play" for DRL agents to effectively reduce carbon emissions through dynamic actions. Additionally, locations with a high average carbon



(a) Alibaba trace 1 v2017 (b) Alibaba trace 2 v2017 (c) Google trace v2011

Figure 6: Examples of different workload traces from Alibaba and Google data centers.

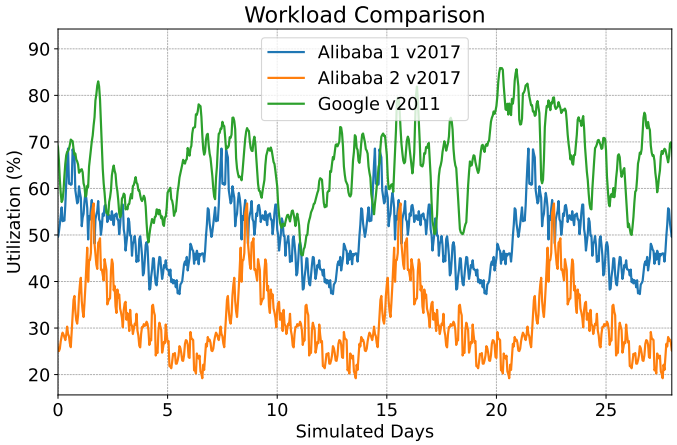
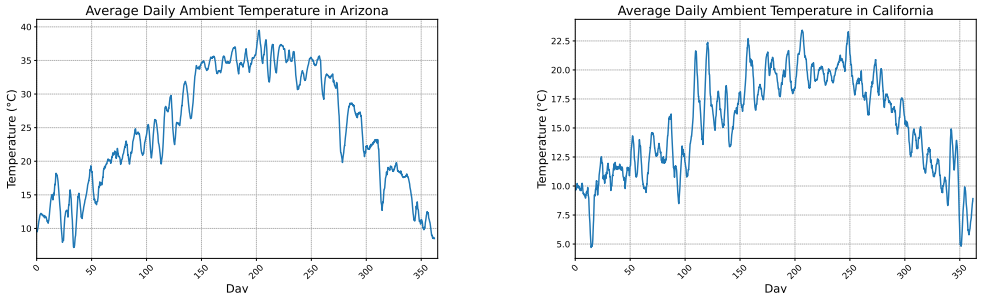
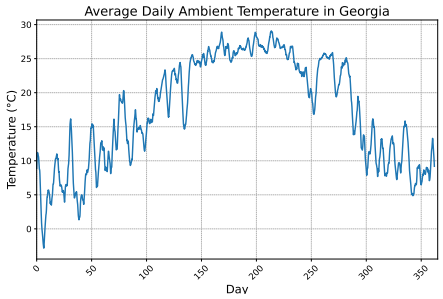


Figure 7: Comparison between two workload traces of Alibaba trace (2017) and Google (2011).

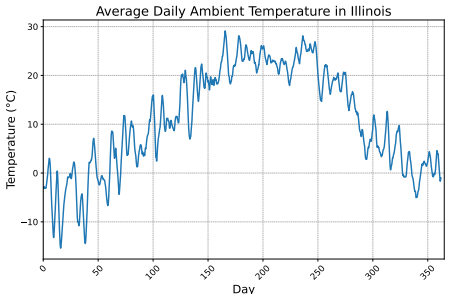


(a) Arizona

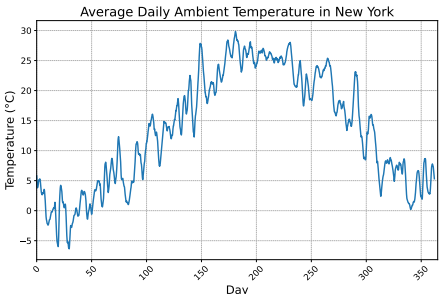
(b) California



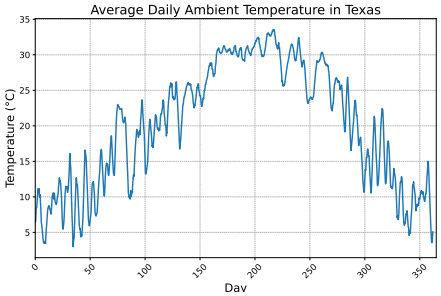
(c) Georgia



(d) Illinois



(e) New York



(f) Texas

Figure 8: Typical average ambient temperature across different locations across one year.

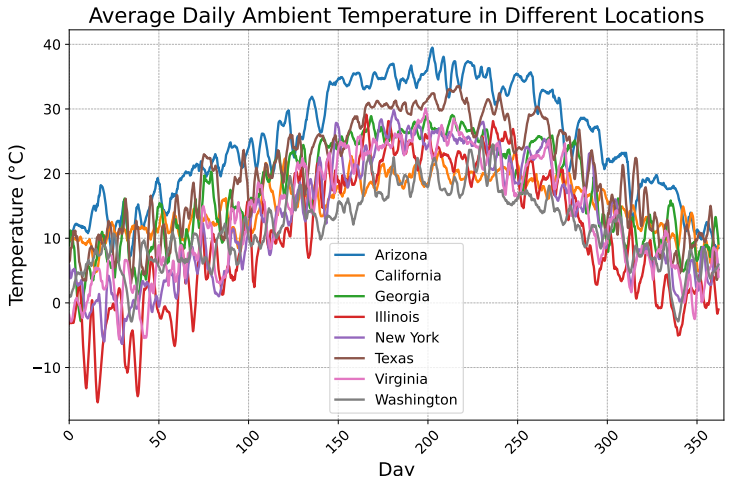


Figure 9: Comparison between external temperature of the different selected locations.

Location	Typical Weather	Carbon Emissions
Arizona	Hot, dry summers; mild winters	High avg CI, High variation
California	Mild, Mediterranean climate	Medium avg CI, Medium variation
Georgia	Hot, humid summers; mild winters	High avg CI, Medium variation
Illinois	Cold winters; hot, humid summers	High avg CI, Medium variation
New York	Cold winters; hot, humid summers	Medium avg CI, Medium variation
Texas	Hot summers; mild winters	Medium avg CI, High variation
Virginia	Mild climate, seasonal variations	Medium avg CI, Medium variation
Washington	Mild, temperate climate; wet winters	Low avg CI, Low variation

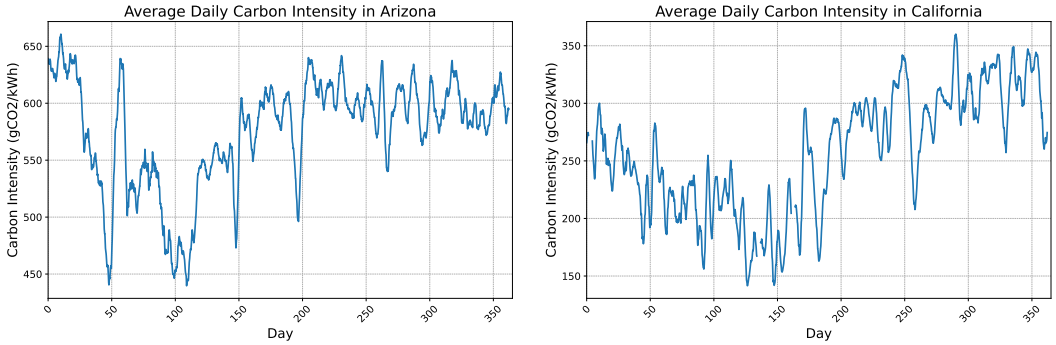
Table 7: Summary of Selected Locations with Typical Weather and Carbon Emissions Characteristics

intensity value present greater opportunities for achieving significant carbon emission reductions. The selected locations are highlighted, while other U.S. locations are also plotted for comparison. Regions with both high CV and high average carbon intensity are identified as prime targets for DRL agents to maximize their impact on reducing carbon emissions.

In the table bellow (7) is the summarizing the selected locations, typical weather values, and carbon emissions characteristics:

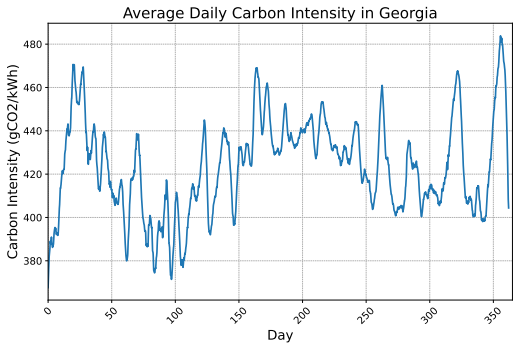
Considering the data from (9), the U.S. states with the highest number of data centers are summarized in Table 8. The states with the most significant number of data centers tend to be Virginia, Texas, California, and New York. Virginia, especially, is a major hub due to its proximity to Washington D.C. and the abundance of fiber optic cable networks. Texas and California are also prominent due to their size, economic output, and significant tech industries. New York, particularly around New York City, hosts numerous data centers that serve the financial sector and other industries.

The selection of these locations is justified by their significant number of data centers, which emphasizes the potential impact of DRL agents in these regions. By targeting areas with both high data center density and favorable carbon intensity characteristics, DRL agents can maximize their effectiveness in reducing carbon emissions.

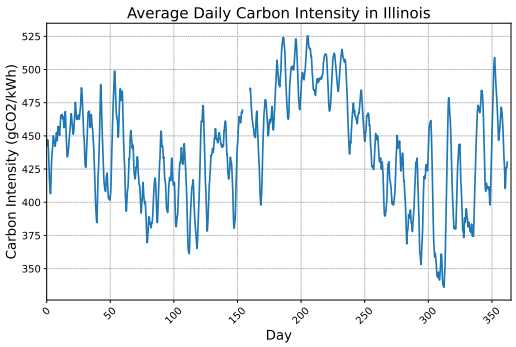


(a) Arizona

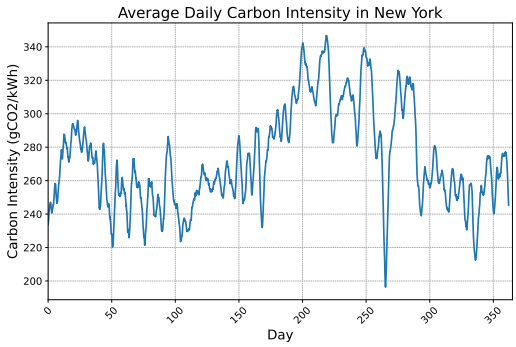
(b) California



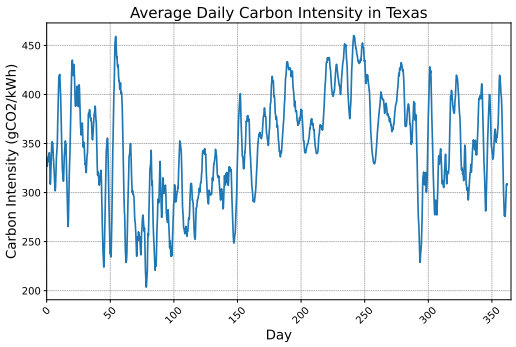
(c) Georgia



(d) Illinois



(e) New York



(f) Texas

Figure 10: Typical average carbon intensity across different locations over one year.

State	Data Centers
California	254
Virginia	250
Texas	239
New York	128
Illinois	122
Florida	120
Ohio	98
Washington	84
Georgia	75
New Jersey	69

Table 8: Summary of U.S. States with the Most Data Centers (ref: (9))

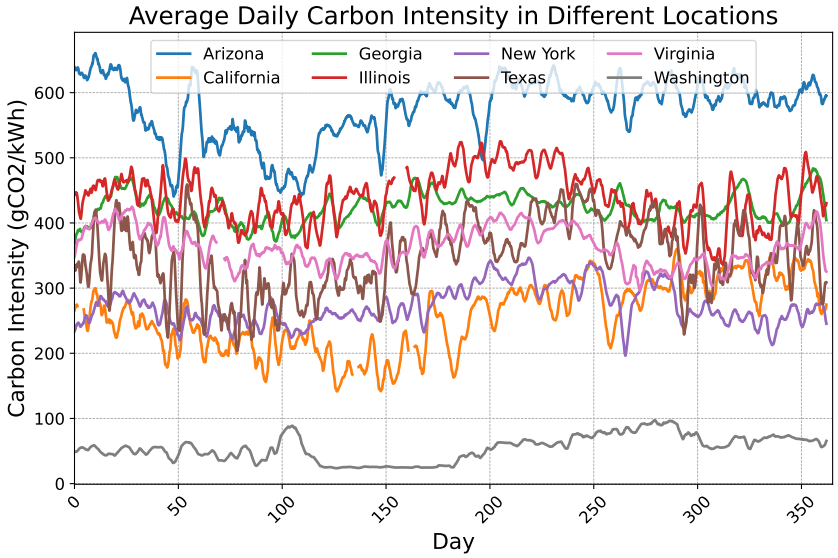


Figure 11: Comparison of carbon intensity across the different selected locations.

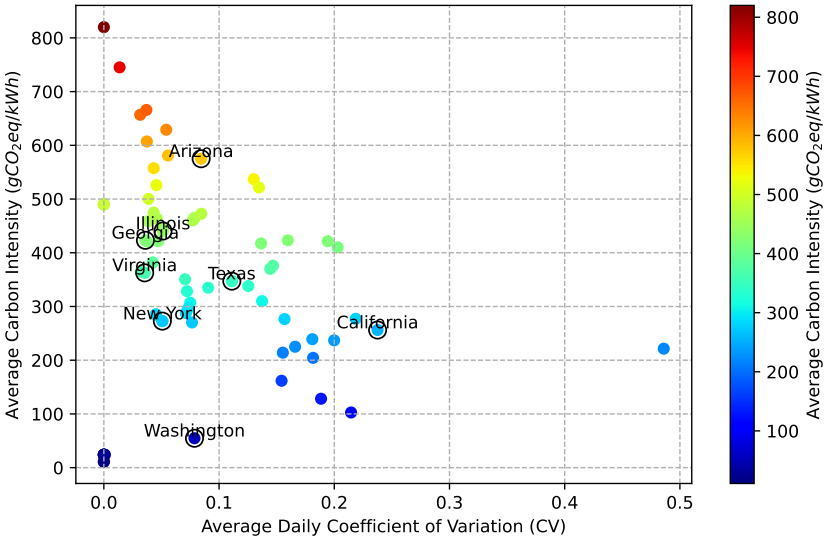


Figure 12: Average daily carbon intensity versus average daily coefficient of variation (CV) for the grid energy provided from US. Selected locations are remarked. High CV indicates more fluctuation, providing more opportunities for DRL agents to reduce carbon emissions. High average carbon intensity values offer greater potential gains for DRL agents.

F Reward Evaluation and Customization

F.1 Load Shifting Penalty ($LS_{Penalty}$)

The Load Shifting Penalty ($LS_{Penalty}$) is applied to the Load Shifting Agent ($Agent_{LS}$) in the Workload Environment (Env_{LS}) if it fails to reschedule flexible workloads within the same day. If D_t (the amount of rescheduled workload left) is positive at the end of the day, $penalty\_tasks\_queue$ is assigned. Additionally, we included a function that progressively increases the penalty as the hour of the day approaches 24h. This means the penalty increases linearly from hour 23h to hour 24h.

Furthermore, there is a penalty for tasks that were dropped due to queue limits ($penalty\_dropped\_tasks$). This penalty is added to discourage the agent from dropping tasks and ensure that workloads are managed efficiently.

Therefore, the $LS_{Penalty}$ is composed of $penalty\_tasks\_queue$ and $penalty\_dropped\_tasks$. Related work in this area include (10; 11; 12; 13; 14; 15; 16).

F.2 Default Reward Function

The default reward function used in SustainDC for the Load Shifting Agent is implemented as follows:

```
def default_ls_reward(params: dict) -> float:
    """
    Calculate the reward value based on normalized load shifting
    and energy consumption.

    Parameters:
        params (dict): Dictionary containing parameters:
            - bat_total_energy_with_battery_KWh (float):
                Total energy consumption with battery.
            - norm_CI (float): Normalized carbon intensity.
            - bat_dcload_min (float): Minimum data center load.
            - bat_dcload_max (float): Maximum data center load.
            - ls_tasks_dropped (int): Number of tasks dropped due to queue limit.
            - ls_tasks_in_queue (int): Number of tasks currently in queue.
            - ls_current_hour (int): Current hour in the simulation.

    Returns:
        float: Calculated reward value.
    """
    # Energy part of the reward
    total_energy_with_battery = params['bat_total_energy_with_battery_KWh']
    norm_CI = params['norm_CI']
    dcload_min = params['bat_dcload_min']
    dcload_max = params['bat_dcload_max']

    # Calculate the reward associated with the energy consumption
    norm_net_dc_load = (total_energy_with_battery - dcload_min) /
                           (dcload_max - dcload_min)
    footprint = -1.0 * norm_CI * norm_net_dc_load

    # Penalize the agent for each task that was dropped due to queue limit
    penalty_per_dropped_task = -10  # Define the penalty value per dropped task
    tasks_dropped = params['ls_tasks_dropped']
    penalty_dropped_tasks = tasks_dropped * penalty_per_dropped_task

    tasks_in_queue = params['ls_tasks_in_queue']
    current_step = params['ls_current_hour']
    penalty_tasks_queue = 0

    if current_step % (24*4) >= (23*4):  # Penalty for queued tasks at the
                                         end of the day
        factor_hour = (current_step % (24*4)) / 96  # min = 0.95833, max = 0.98953
        factor_hour = (factor_hour - 0.95833) / (0.98935 - 0.95833)
        penalty_tasks_queue = -1.0 * factor_hour * tasks_in_queue / 10  # Penalty
                                                  for each task left in the queue

    LS_penalty = penalty_dropped_tasks + penalty_tasks_queue
```

```
    reward = footprint + LS_penalty

    return reward
```

F.3 Customization of Reward Formulations

Users can choose to use any other reward formulation by defining custom reward functions inside *utils/reward_creator.py*. To create a custom reward function, you can define it as follows:

```
def custom_reward(params: dict) -> float:
    # Custom reward calculation logic
    pass
```

Replace the logic inside the `custom_reward` function with your custom reward logic.

For more examples of custom reward functions, users can check the file *utils/reward_creator.py*.

To use the custom reward function, you need to include it in the *utils/reward_creator.py* as follows:

```
# Other reward methods can be added here.

REWARD_METHOD_MAP = {
    'default_dc_reward' : default_dc_reward,
    'default_bat_reward': default_bat_reward,
    'default_ls_reward' : default_ls_reward,
    # Add custom reward methods here
    'custom_reward' : custom_reward,
}
```

Additionally, you need to specify the reward function in *harl/configs/envs_cfgs/dcrl.yaml*:

```
agents:
...
ls_reward: default_ls_reward
dc_reward: default_dc_reward
bat_reward: default_bat_reward
...
```

This flexibility ensures that SustainDC can be adapted to a wide range of research and operational needs in sustainable data center management.

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