Comprehensive Link-Level Simulator for Terahertz MIMO Integrated Sensing and Communication Systems with TDD Framework

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Abstract—Terahertz (THz) integrated sensing and communication (ISAC) with multiple-input multiple-output (MIMO) architecture is recognized as a promising interdisciplinary technology for ultra-high-rate mobile communications since the systems enable narrow beam tracking which is necessary in the THz band. In this work, a link-level simulator for THz MIMO ISAC in time-division duplex (TDD) operation is proposed to design and analyze mobile systems. Compared to the simulators in the literature, the proposed simulator is more practical and comprehensive, employing two-dimensional motion simulation instead of numerical evaluation, and considering THz characteristics such as wideband echo, multipath components and molecular absorption. Specifically, the simulator supports the standard orthogonal frequency division multiplexing (OFDM) and discrete Fourier transform spread OFDM (DFT-s-OFDM) waveforms for sensing and communication simultaneously. Trade-offs between communication and sensing metrics required for waveform numerology design are investigated. In particular, by exploiting TDD framework’s integration capability, range-velocity-angle estimation with virtual array and sensing-aided downlink spatial multiplexing are co-designed. Additionally, a user interface with elaborate parameter configuration is introduced. Finally, we implement an urban vehicle-to-vehicle (V2V) application case to verify the simulator. The simulation results present the feasibility of the developed integrated architecture.

Index Terms—THz ISAC, MIMO, TDD, OFDM waveform numerology, link-level simulator.

I. INTRODUCTION

The terahertz (THz) band (0.1-10 THz), the last unutilized piece of radio-frequency (RF) spectrum [1], where hundreds of GHz bandwidth is available to facilitate wireless transmission of terabit-per-second (Tbps) rates, is recognized as one of the candidate bands and key technologies for the sixth generation (6G) of mobile communication systems by academia and industry worldwide [2], [3]. Aiming to realize the comprehensive interconnection of man-machine-thing in 6G, THz integrated sensing and communication (ISAC) is promoted recently [4].

On one hand, ultra-fast links and ultra-accurate sensing become a reality thanks to the ultra-broad bandwidth in the THz band. On the other hand, due to the short wavelength of THz wave, smaller antennas are expected to be equipped with area and cost-sensitive infrastructures. In addition, the non-ionization and penetrability of THz wave facilitate safe detection and imaging, enabling portable and wearable devices. Furthermore, to keep up with 6G requirements in mobile services, THz ISAC presents a trend of transformation from static cases and single-input-single-output (SISO) to mobile applications and multiple-input-multiple-output (MIMO) that enables to overcome the limitation in THz propagation distances. Therefore, THz MIMO ISAC is envisioned for various applications in 6G, such as THz localization [5], THz extended reality (XR) [6], Tbps Internet-of-Things (IoT) [7], and THz-assisted vehicle-to-everything (V2X) networks [8].

There are various classes of hot topics for THz MIMO ISAC in the literature, including power-efficient transceiver design [9], channel measurement and modeling [10], waveform and beamforming design [11], simulator development at different levels [12], etc. Among these researches, simulation platform is the prerequisite for all novel systems to be deployed in real-world scenarios. It is because simulators provide a necessary and efficient way to design and evaluate new technologies and applications. Therefore, it is vital to develop a THz ISAC simulator appropriate for MIMO and mobile applications.

Over the past few years, a number of THz, ISAC, and THz ISAC system simulators have been released [13]–[19]. TeraSim [13] is an ns-3 extension for system-level testing of THz networking protocols, implementing physical and medium access control layer solutions. As an early release simulator, it only covers line-of-sight (LoS) scenarios and does not support waveform evaluation. TeraMIMO [14] and BUPTCMG-IMT2030 THz [15] are statistical three-dimensional (3D) THz channel simulators, the former based on wideband ultra-massive MIMO architecture and supporting both LoS and non line-of-sight (NLoS) scenarios, the latter based on International Telecommunications Union-Radio Communications Sector (ITU-R) M.2412 standard framework and focusing on modeling various indoor and outdoor scenarios at the sub-THz band. However, in a similar context, both are channel modeling platforms without the ability to test THz
communication and sensing techniques. In [16], a new module of the Simulator for Mobile Networks (SiMoNe) is presented, considering single-carrier (SC) physical layer design based on IEEE 802.15.3d standard, but not compatible with multi-carrier (MC) modulation, MIMO, and ISAC, and thus has poor applicability to 6G systems. Even though some of the ISAC simulators as in [17], [18] support sensing or localization algorithms, they only work in the Sub-6GHz and millimeter-wave bands and hence unable to simulate THz-specific signal processing and propagation characteristics.

Most notably, TeraISAC [19], a lately published THz ISAC link-level simulator, supports a variety of air-interface waveforms, including orthogonal frequency division multiplexing (OFDM) and discrete Fourier transform spread OFDM (DFT-s-OFDM) with lower peak-to-average power ratio (PAPR) that are regarded as potential modulation schemes for 6G THz ISAC [20]. The waveform numerologies supported in the simulator follow the latest standardization work on the evolution of 5G New Radio (NR) [21]. Nevertheless, when it comes to various ISAC scenarios, the fixed frame structure cannot simultaneously meet differentiated requirements. In addition, TeraISAC essentially supports only a communication-centric coexistence system without designing a specific duplex operating scheme to converge sensing and communication. Subsequently, it is limited to SISO systems at 140 GHz and 300 GHz without angle estimation capabilities, which limits the applicability, and it does not consider the influence of terahertz wideband effect on the sensing model. To the best of our knowledge, there have been no specialized THz simulators that simultaneously consider overall ISAC framework, MIMO architecture, and THz characteristics in both communication and sensing cases. This motivates our work.

This paper constructs a comprehensive link-level simulator with waveform numerology design guidelines for THz MIMO ISAC systems. In particular, the simulator can utilize the time-division duplex (TDD)-based ISAC framework to simultaneously perform sensing and communication based on OFDM and DFT-s-OFDM. It also supports THz characteristics modeling and elaborate parameters configuration. The detailed comparisons of the proposed simulator with the existing THz and ISAC simulators are listed in Table I. The main contributions of this work are summarized below:

1) A link-level simulator for THz MIMO ISAC systems is developed. TDD framework, colocated MIMO system, multi-antenna user equipment (UE), OFDM and DFT-s-OFDM waveforms, and fine-grained parameters configuration for entire systems are supported. Moreover, THz peculiarities, including wideband echo model, exhauster molecular absorption loss, and LoS-dominant and NLoS-assisted communication channel, are captured.

2) In the simulator architecture, TDD-based ISAC framework and virtual sum coarray techniques are unified, based on which we implement different precoding approaches during the sensing and communication periods to integrate virtual array estimation and multi-stream transmission with Doppler compensation and THz beam alignment enhancement.

3) A time-varying 2D motion mechanism realistically simulating the movements in practical systems is employed instead of numerical computations.

4) Trade-offs between communication and sensing metrics are studied from the waveform perspective, based on which general design guidelines for OFDM and DFT-s-OFDM numerology are proposed to satisfy the varying

<table>
<thead>
<tr>
<th>Simulators</th>
<th>Publication</th>
<th>General profile</th>
<th>Type</th>
<th>THz</th>
<th>ISAC</th>
<th>MIMO</th>
<th>Mobility</th>
<th>THz characteristics considered</th>
</tr>
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<tr>
<td>TeraSim [13]</td>
<td>ELSEVIER NCN 2018</td>
<td>Simulation platform for THz nanoscale/macroscopic communication networks</td>
<td>System level</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Static</td>
<td>Frequency selective electromagnetic model only covering LoS</td>
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<tr>
<td>TeraMIMO [14]</td>
<td>IEEE TVT 2021</td>
<td>Provide a 3D THz-specific channel model covering LoS and NLoS communications</td>
<td>Channel level</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Static</td>
<td>Cluster-based statistical wideband UM-MIMO THz channel at 100-550 GHz</td>
</tr>
<tr>
<td>BUPTCMG-IMT2030 THz [15]</td>
<td>arXiv preprint 2023</td>
<td>IMT2030-based THz channel simulation platform towards 6G</td>
<td>Channel level</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Static</td>
<td>Measurement-based sub-THz channel model supporting spatial non-stationary</td>
</tr>
<tr>
<td>SiMoNe [16]</td>
<td>AGU RDS 2022</td>
<td>A modular physical layer simulator for THz communication systems</td>
<td>Link level</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Static</td>
<td>3D raytracing-based model operating in IEEE 802.15.3d for city or indoor scenarios</td>
</tr>
<tr>
<td>HermesPy [17]</td>
<td>IEEE Access 2022</td>
<td>6G multi-node joint communications and sensing scenarios evaluation</td>
<td>Link level</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Static</td>
<td>N/A</td>
</tr>
<tr>
<td>5G localization simulator [18]</td>
<td>IEEE TWC 2023</td>
<td>Detect physical behaviors of the 5G positioning signal considering real IM transmission</td>
<td>Link level</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Static</td>
<td>N/A</td>
</tr>
<tr>
<td>TeraISAC [19]</td>
<td>GitHub 2023</td>
<td>Evaluate performance of simplified THz SISO ISAC systems in mid-range</td>
<td>Link level</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Numerical evaluation</td>
<td>Molecular absorption coefficient at 140 and 300 GHz</td>
</tr>
<tr>
<td>This work</td>
<td>N/A</td>
<td>THz MIMO ISAC simulator co-designing TDD-based sensing-aided scheme and virtual array estimation</td>
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<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>2D motion simulation</td>
<td>Wideband echo model, Molecular absorption loss, and modified SV model</td>
</tr>
</tbody>
</table>

This work considers the applicability and it does not consider the influence of terahertz wideband effect on the sensing model. To the best of our knowledge, there have been no specialized THz simulators that simultaneously consider overall ISAC framework, MIMO architecture, and THz characteristics in both communication and sensing cases. This motivates our work.
requirements of different applications.
5) For more user-friendly operation, an efficient user interface (UI) with parameters setting and performance visualization is introduced.
6) An urban vehicle-to-vehicle (V2V) application case and its simulation results are presented to verify the capabilities of the simulator, and to evaluate the performance of OFDM and DFT-s-OFDM in THz MIMO ISAC.

The rest of this paper is organized as follows: Section II sketches the ISAC transmission framework. Section III presents the THz MIMO ISAC system model. In Section IV, we propose the waveform numerology design guidelines for THz ISAC. Section V specifies the simulator architecture and its UI. Section VI presents the urban V2V application case and the corresponding simulation results. Finally, Section VII concludes the paper and provides a vision for future works.

Notations: lower case, bold lower case, and bold upper case letters correspond to scalars, vectors, and matrices, respectively. $\mathbb{C}$ denotes the set of complex numbers, and $\otimes$ denotes the element-wise Hadamard product. $0_{M \times N}$ and $I_{M \times N}$ represent $M \times N$ zero and $M \times N$ one matrices, respectively, and $I_M$ is a $M \times M$ identity matrix. The superscripts $(\cdot)^T$ and $(\cdot)^H$ stand for the transpose and conjugate transpose functions, respectively. $\operatorname{diag}(\cdot)$ and $\operatorname{vec}(\cdot)$ denote a diagonal matrix and matrix vectorization operator, respectively. $\operatorname{reshape}_{M \times N}(\cdot)$ reshapes a vector or matrix into a $M \times N$ matrix column-wise. We use $\mathcal{F}\{\cdot\}$ to denote the Fourier transform, $\mathcal{E}[\cdot]$ the expectation, $| \cdot |$ the modulus, and $\| \cdot \|_F$ the Frobenius norm of a set. $\mathcal{CN}(\mu, \sigma^2)$ is a complex Gaussian random variable with mean $\mu$ and variance $\sigma^2$, and $\mathcal{U}(a, b)$ is a real uniform random variable with lower bound $a$ and upper bound $b$.

II. TDD-BASED ISAC TRANSMISSION FRAMEWORK

Inspired by MIMO radars, we unify the novel TDD-based ISAC framework proposed in [22] and proven virtual sum coarray techniques in [23], which aims to assist THz beam alignment with higher angular estimation accuracy substituting for conventional beam training schemes with high overhead. As shown in Fig. 1, the adopted transmission framework is generally split into the following three periods:

1) UE searching, sensing, and communication channel estimation: Initially, the ISAC system has no a priori knowledge about the UE, in this case the ISAC system first transmits preamble signals in the field of view (FOV) to search for the UE and to estimate the communication channel, and then successively receives the echo signal and the uplink (UL) feedback signal from the UE. Since the echo is reflected instantaneously after hitting the UE, the resulting round-trip delay is typically shorter than the processing delay of the UL communication, as a result, the echo is assumed to always arrive ahead of the UL transmission. Despite this, a guard period is required between downlink (DL) and UL to avoid the interference between UL signals and target echoes. In details, after receiving the echo from the UE, the ISAC system estimates its range, relative radial velocity, and azimuth angle to achieve UE sensing. Besides, the UE also receives the preamble signals through multipaths (MPs), based on which it estimates the DL communication channel and feeds the channel frequency response (CFR) estimation back to the ISAC system via UL signals.

2) Sensing-aided DL communication: In Period 2, based on the estimates and UL feedback in Period 1, the ISAC system transmits data with precoding, pre-compensating the Doppler shift, and formulating directional DL beams towards the UE, aiming to implement sensing-aided communication.

3) UE tracking and UL communication: After Period 2, the ISAC system will receive the echo of the DL data signal and the UL data signal form the UE, and the ISAC system may tracks the variation of the UE while decoding the UL information. In Period 3, similarly, we still reserve a guard period between DL and UL operations to guarantee transmission without collisions.

In this work, our main interests are Period 1 and Period 2, i.e., UE sensing and sensing-aided communication. As such, in what follows, we will only elaborate the system model during these two periods.

III. THZ MIMO ISAC SYSTEM MODEL

We consider a colocated THz MIMO ISAC system formed by $N_{\text{Tx}}^{\text{ISAC}}$ transmit (Tx) antennas and $N_{\text{Rx}}^{\text{ISAC}}$ receive (Rx) antennas and a single UE with $N_{\text{UE}}$ antennas (usually supposing $N_{\text{UE}} \leq N_{\text{ISAC}}^{\text{TX}}$). Both the ISAC system and UE are equipped with digital uniform linear arrays (ULAs). Specially, the ISAC system’s transceiver is configured with a sparse Tx ULA and a filled Rx ULA which enables constructing a virtual filled ULA of $N_{\text{ISAC}}^{\text{TX}} N_{\text{ISAC}}^{\text{RX}}$ elements (Fig. 1) via time-division multiplexing (TDM) approach [24] during the sensing period. For convenience, we designate the centers of the Tx/Rx ULAs of the ISAC system to be colocated at the origin of the global 2D Cartesian coordinate systems, i.e., $p_{\text{ISAC}} = [0, 0]^T$. In this section, following the ISAC framework structure in Section II, we propose a MIMO-(DFT-s-)OFDM transmission scheme, and derive the corresponding transceiver signal models.

A. THz TDM-MIMO Sensing Model

In the first period, the ISAC system transmits the OFDM/DFT-s-OFDM preamble signals within the FOV. For the duration of consecutive $N_{\text{sym}}$ symbols, the preamble signal has a total bandwidth $B = N_c \Delta f$ and total frame duration $T_f = N_{\text{sym}} T_{\text{sym}}$, where $N_c$ and $\Delta f$ denote the number of subcarriers and the subcarrier spacing, respectively. $T_{\text{sym}} = T_{\text{CP}} + T_{\text{u}}$ represents the entire symbol duration, $T_{\text{CP}}$ and $T_{\text{u}} = 1/\Delta f$ is the cyclic prefix (CP) duration and the effective symbol duration, respectively.

First, let $X_b \in \mathbb{C}^{N_c \times N_{\text{sym}}}$ be the 2D data grid mapped by transmit bit streams through the preamble sequence. In contrast with OFDM, before mapping this grid to the time-frequency (TF) plane, DFT-s-OFDM performs an additional $N_c$-point DFT spreading operation (i.e., the spreading factor is one to keep the same spectral efficiency as OFDM) to significantly reduce the PAPR. So, the OFDM/DFT-s-OFDM grid in the TF domain is given by

$$X^{\text{TF}} = \begin{cases} X_b, & \text{for OFDM} \\ F_{N_c} X_b, & \text{for DFT-s-OFDM} \end{cases},$$

where $F_{N_c}$ denotes the $N_c$-point DFT operation.
where \( \{X^{TF}\}_{n,m} \) denotes the frequency tone on the \( m \)-th subcarrier for the \( n \)-th symbol, and \( \mathbf{F}_{\text{ISAC}} \subseteq \mathbb{C}^{N_{\text{Tx}} \times N_{\text{sym}}} \) is a unitary DFT matrix with \( [\mathbf{F}_{\text{ISAC}}]_{n,k} = \frac{1}{\sqrt{N_{\text{sym}}}} e^{-j2\pi nk/N_{\text{sym}}} \). In order to form a virtual array at the receiver of the ISAC system, we use the virtual array approach to ensure mutually orthogonal transmit waveforms, and then the precoded (DFT-s-)OFDM grid transmitted by the \( i \)-th Tx antenna is represented as

\[
X_i^{TF} = X^{TF} \otimes F_i^{sen} \subseteq \mathbb{C}^{N_{\text{sym}} \times N_{\text{sym}}},
\]

where \( F_i^{sen} \subseteq \mathbb{C}^{N_{\text{sym}} \times N_{\text{sym}}} \) represents the symbol-wise TDM precoding matrix, satisfying the following constraints: (i) \( F_i^{sen} \otimes F_j^{sen} = 0_{N_{\text{sym}} \times N_{\text{sym}}} \), \( i \neq j \); (ii) \( \sum_{i=1}^{N_{\text{ISAC}}} \sum_{j=1}^{N_{\text{ISAC}}} \mathbf{F}_i^{sen} = 1_{N_{\text{sym}} \times N_{\text{sym}}} \); (iii) \( \sum_{i=1}^{N_{\text{ISAC}}} \|F_i^{sen}\|^2 = N_{\text{ISAC}} \).

Next, applying the inverse fast Fourier transform (IFFT) to map the TF domain preamble grid \( X_i^{TF} \) to time domain, the complex baseband time domain OFDM/DFT-s-OFDM signal for the \( i \)-th Tx antenna after the CP addition is given by

\[
s_i(t) = \frac{1}{\sqrt{N_{\text{sym}}}} \sum_{n=0}^{N_{\text{sym}}-1} \sum_{m=0}^{N_{\text{sym}}-1} [X_i^{TF}]_{n,m} e^{j2\pi n \Delta f (t-mT_{\text{sym}})} e^{{\text{rect}}\left(\frac{t}{T_{\text{CP}}} - 1\right)},
\]

where \( \text{rect}(\cdot) \) is the rectangular function defined as

\[
\text{rect}\left(\frac{t}{T}\right) = \begin{cases} 1, & \text{for } 0 \leq t < T, \\ 0, & \text{otherwise}. \end{cases}
\]

Finally, after upconversion, the time domain RF signal transmitted over all Tx antenna elements for the entire frame is written as

\[
s(t) = [s_1(t), \ldots, s_{N_{\text{ISAC}}}^{N_{\text{ISAC}}}](t) e^{j2\pi f_c t} \subseteq \mathbb{C}^{N_{\text{Tx}} \times 1}.
\]

In this work, the ISAC system has a 2D absolute velocity of \( v_{\text{ISAC}} = [v_x^{\text{ISAC}}, v_y^{\text{ISAC}}] \), and the single UE is assumed to be regarded as a point target in the far-field on LoS, characterized by a range \( r \) at \( t = 0 \), a relative velocity \( v \) (supposing \( |v| \ll c_0 \)), and a Doppler shift \( \nu_{\text{sen}} = 2v/\lambda \), with \( c_0 \) and \( \lambda = c_0/f_c \) being the speed of light and the carrier wavelength, respectively. During the simulation, both the ISAC system and the UE dynamically update their positions every symbol length \( T_{\text{sym}} \), and \( a_{\text{ISAC}} \) denote the respective steering vectors of the Tx and Rx ULAs of the ISAC system, i.e.,

\[
\mathbf{a}_{\text{Tx}}^{\text{ISAC}}(\theta) = \left[ e^{j2\pi f_{\text{sym}}(N_{\text{ISAC}}-1)/2T_{\text{sym}}} \left( \frac{N_{\text{ISAC}}}{2} \right) \right],
\]

\[
\mathbf{a}_{\text{Rx}}^{\text{ISAC}}(\theta) = \left[ e^{j2\pi (N_{\text{sym}}T_{\text{sym}}/2) - j2\pi f_{\text{sym}}(N_{\text{ISAC}}-1)/2T_{\text{sym}}} \left( \frac{N_{\text{ISAC}}}{2} \right) \right],
\]

where \( d_{\text{Tx}} = N_{\text{ISAC}} \lambda/2 \) and \( d_{\text{Rx}} = \lambda/2 \) denote the Tx and Rx antenna spacing, respectively.

Due to the large time-bandwidth product (TBP) of the THz OFDM signals, i.e. \( B_T \ll c_0/2|v| \), the time stretching/compression of the echo signal caused by the Doppler effect cannot be neglected [25]. Hence, the wideband time-varying MIMO sensing channel model \( \mathbf{H}_{\text{sen}} \subseteq \mathbb{C}^{N_{\text{ISAC}} \times N_{\text{Tx}}} \) can be written by [26], [27]

\[
\mathbf{H}_{\text{sen}}(t, \tau) = \alpha_{\text{sen}} \sqrt{\delta(\tau - \tau_{\text{sen}})} e^{j2\pi f_{\text{sym}}d} G_{\text{ISAC}}(\theta) G_{\text{Rx}}^{\text{ISAC}}(\theta) a_{\text{ISAC}}(\theta) a_{\text{ISAC}}^H(\theta),
\]
where $\gamma = 1 + 2v/c_0$ represents the stretching or compressing in time of the echo signal with $\beta = 2v/c_0$ being the Doppler-spread factor, $G_{\text{ISAC}}(\cdot)$ and $G_{\text{Rx}}(\cdot)$ are the Tx and Rx antenna gains, respectively. Considering the more significant of the UE, and $\alpha$ denotes the path loss exponent (PLE), whose best fit value is around 2 in the THz band according to measurement-based works [29], [30], $\sigma_{\text{RCS}}$ is the radar cross-section (RCS) of the UE, and $-K(f_c)e^{\gamma}$ accounts for the round-trip molecular absorption loss, with $K(f_c)$ denoting the frequency-dependent molecular absorption coefficient. The calculation of $K$ involves parameters of each gas and isotropotropy in the atmosphere, which can be derived from [31] in detail.

Based on the above sensing channel model, the echo signal received by the ISAC system is expressed as

$$y_{\text{sen}}(t) = \int H_{\text{sen}}(t, \tau)s(t - \tau)d\tau + n_{\text{sen}}(t) = \alpha_{\text{sen}}\sqrt{\frac{4\pi\sigma_{\text{RCS}}}{\lambda^2}}G_{\text{ISAC}}(\theta)G_{\text{Rx}}(\theta)\hat{a}_{\text{ISAC}}^T(\theta) \cdot \hat{a}_{\text{ISAC}}^T(\theta)\mathbf{s}(\gamma(t - \tau_{\text{sen}}) + n_{\text{sen}}(t)), \quad (10)$$

where $n_{\text{sen}}(t) \in \mathbb{C}^{N_{\text{ISAC}} \times 1}$ is the additive white Gaussian noise (AWGN) in sensing model, with the total noise power calculated by $\sigma_{\text{sen}}^2 = \mathbb{E}_t[T_{\text{sym}}B_{\text{ISAC}}^2]$, where $\mathbb{E}_t$ denotes the Boltzmann constant, $T_{\text{sym}}$ and $N_{\text{ISAC}}$ refer to the system thermal noise temperature and the receiver noise figure of the ISAC system, respectively.

### B. 3D-FFT-Based Estimation Algorithm

Before formulating the echo signal in a compact form, we generally make the following standard assumptions [32], [33]: (i) the CP duration is properly chosen to satisfy $T_{\text{CP}} \geq \tau_{\text{sen}}$; (ii) the Doppler-spread factor $\beta$ satisfies $|\beta| \ll 1/N_c$. Under this setting, sampling $y_{\text{sen}}(t)$ at $t = mT_{\text{sym}} + \mu T_{\text{sym}}/N_c$, $\mu = 0, 1, \ldots, N_c - 1$ after CP removal per symbol and downconversion, the discrete-time expression of the time-averaging terms in (10) can be obtained by [32]-[34]

$$\mathbf{y} = \mathbf{H} = \mathbf{a}_{\text{ISAC}}^T(\theta)\mathbf{s}(\gamma(t - \tau_{\text{sen}}))|_{t=mT_{\text{sym}}+T_{\text{CP}}+\mu T_{\text{sym}}/N_c} = \sum_{j=1}^{N_{\text{ISAC}}}[\mathbf{a}_{\text{ISAC}}^T(\theta)]^j \mathbf{F}^H(\mathbf{d}(\beta) \circ \mathbf{s}_i \circ \mathbf{b}(\tau_{\text{sen}})) \circ \mathbf{c}(\tau_{\text{sen}}), \quad (11)$$

where $\mathbf{F} \in \mathbb{C}^{N_cN_{\text{sym}} \times N_{\text{sym}}}$ is a unitary DFT matrix, and $\mathbf{s}_i \in \mathbb{C}^{N_cN_{\text{sym}} \times 1}$ is the sampled representation of $s_i(t)$ in (3). For convenience of expression, respectively, the frequency-domain and temporal steering vectors and the inter-subcarrier Doppler effect matrix are defined as

$$\mathbf{b}(\tau) = \mathbf{b}_{N_c}(\tau) \otimes 1_{N_{\text{sym}}} \in \mathbb{C}^{N_cN_{\text{sym}} \times 1}, \quad \mathbf{c}(\nu) = \mathbf{c}_{N_{\text{sym}}}(\nu) \otimes 1_{N_{\text{sym}} \times 1}, \quad \mathbf{d}(\beta) = \text{reshape}_{N_cN_{\text{sym}} \times 1}(\tilde{\mathbf{d}}(\beta)) \in \mathbb{C}^{N_cN_{\text{sym}} \times 1}, \quad (12)$$

where $\mathbf{b}(\tau)$ denotes the frequency-domain steering vector with $\mathbf{b}_{N_c}(\tau) \triangleq \left[1, e^{-j2\pi\Delta fT_c}, \ldots, e^{-j2\pi(N_c-1)\Delta fT_c}\right] \in \mathbb{C}^{N_c \times 1}$ [33], $\mathbf{c}(\nu)$ denotes the temporal steering vector with $\mathbf{c}_{N_{\text{sym}}}(\nu) \triangleq \left[1, e^{-j2\pi T_{\text{sym}}\nu}, \ldots, e^{-j2\pi(N_{\text{sym}}-1)T_{\text{sym}}\nu}\right] \in \mathbb{C}^{N_{\text{sym}} \times 1}$ and $\mathbf{c}_{T_{\text{sym}}}(\nu) \triangleq \left[1, e^{-j2\pi T_{\text{sym}}\nu}, \ldots, e^{-j2\pi(N_{\text{sym}}-1)T_{\text{sym}}\nu}\right] \in \mathbb{C}^{N_{\text{sym}} \times 1}$ [34], and $\mathbf{d}(\beta)$ is the inter-subcarrier Doppler effect matrix which reshapes $\mathbf{d}(\beta) \in \mathbb{C}^{N_c \times N_{\text{sym}}} \times 1$ matrix column-wise with $\mathbf{d}(\beta)|_{m,n} \triangleq e^{j2\pi\beta(m+1+\alpha)}$ for $n = 0, 1, \ldots, N_c - 1, m = 0, 1, \ldots, N_{\text{sym}} - 1$ [32], $\alpha = T_{\text{CP}}/T_u$ is the ratio of the CP duration to the effective symbol duration.

Synthesize all the above decompositions, plugging (11)-(14) yields the discrete time-space representation of the received signal in the sensing model arranged by

$$\mathbf{Y} = \mathbf{a}_{\text{ISAC}}(\nu_{\text{sen}})\mathbf{F}^H\mathbf{D}(\beta)\mathbf{B}(\tau_{\text{sen}})\mathbf{S}_{\text{ISAC}}(\theta)\mathbf{a}_{\text{ISAC}}^T(\theta) + \mathbf{N}, \quad \mathbf{N} = \mathbb{C}^{N_cN_{\text{sym}} \times N_{\text{sym}} \times N_{\text{sym}}}, \quad (15)$$

where $\mathbf{D}(\beta) \triangleq \text{diag}(\mathbf{d}(\beta)) \in \mathbb{C}^{N_{\text{sym}} \times N_{\text{sym}}}$, $\mathbf{B}(\tau_{\text{sen}}) \triangleq \text{diag}(\mathbf{b}(\tau_{\text{sen}})) \in \mathbb{C}^{N_{\text{sym}} \times N_{\text{sym}}}$. The ISAC system decodes received echo signals by separating the $N_{\text{sym}}$ transmit waveforms at each of its $N_{\text{sym}}$ Rx antennas to form a virtual array of size $N_{\text{virt}} = N_{\text{sym}}^2N_{\text{sym}}$ Rx, and the decoded 3D data cube can be written by

$$\mathbf{Y} = \text{reshape}_{N_cN_{\text{sym}} \times N_{\text{sym}}} \left(\mathbf{Y}/\mathbf{S}\right) \in \mathbb{C}^{N_c \times N_{\text{sym}} \times N_{\text{sym}}}, \quad (16)$$

where the number of symbols in time domain becomes equivalent to $N_{\text{sym}} = N_{\text{sym}}/N_{\text{ISAC}}$.

Afterward, FFT is operated on the three dimensions of this cube in sequence. Firstly, the range FFT implemented on symbol $m$ and virtual array element $q$ is given by $\mathbf{Y}_R|_{n,m,q} = \mathcal{F}([\mathbf{Y}|_{n,m,q}]$, with $n_{\text{virt}}$ being the range bin, yields the range resolution $\Delta r = \frac{v}{2N_{\text{sym}}}2\pi$ and the range estimation $\hat{r} = k\Delta r, k = 0, 1, \ldots, N_{\text{sym}} - 1$. Secondly, velocity FFT is applied on the obtained range profile that generates the range-velocity (RV) map expressed by $\mathbf{Y}_R|_{n,v_{\text{Rx}},m,q} = \mathcal{F}([\mathbf{Y}_R|_{n,m,q}]$, where $m_{\text{Rx}}$ denotes the relative radial velocity bin, the velocity resolution is given by $\Delta v = \frac{\hat{v}}{2N_{\text{sym}}}2\pi$ and the velocity estimation result is $\hat{v} = \frac{q}{r}v, p = -N_{\text{sym}}/2, 0, \ldots, N_{\text{sym}}/2 - 1$. At last, the azimuth angle estimation is executed by angle FFT over the virtual array elements, thus the range-velocity-angle (RVA) map is represented by $\mathbf{Y}_{\text{RVA}}|_{n,m,v_{\text{Rx}},q} = \mathcal{F}([\mathbf{Y}_R|_{n,m,q}]$, with $q$ being the azimuth angle bin. Compared with traditional MIMO systems, the angle resolution with TDM coding is improved by $N_{\text{ISAC}}^2$ times, given by $\Delta \theta = 2\sin^{-1}(\frac{1}{N_{\text{sym}}}) \cos \frac{\hat{\theta}}{N_{\text{sym}}}$ [35]. Therefore, the angle estimation result is calculated as $\hat{\theta} = 2q\sin^{-1}(\frac{1}{N_{\text{sym}}}), q = -N_{\text{virt}}/2, 0, \ldots, N_{\text{virt}}/2 - 1$. 


C. THz Communication Channel Model

Different from the sensing channel model that only considers the LoS path, the THz communication channels are usually LoS-dominant and NLoS-assisted. Thus, we adopt a modified Saleh-Valenzuela (SV) model to characterize the THz-specific MP components, and the THz MIMO communication channel \(H_{\text{com}} \in \mathbb{C}^{N_{\text{Rx}} \times N_{\text{ISAC}}} \) can be modeled as [36]

\[
H_{\text{com}}(t, \tau) = \alpha_{\text{com}} \delta(t - \tau_{\text{LoS}}) e^{j2\pi f_{\text{com}} t} G_{\text{ISAC}}(\phi_Tx) \\
+ \sum_{c=1}^{N_{\text{clus}}} \sum_{\ell=1}^{N_{s}} \alpha_{c,\ell} N_{\text{LoS}}(\tau - \tau_{\text{LoS}}) e^{j2\pi f_{\text{com}} \tau} G_{\text{ISAC}}(\phi_{c,\ell}),
\]

(17)

where \(\alpha_{\text{com}}\) and \(N_{\text{LoS}}\) denote the path gains of the LoS and NLoS rays, \(\nu_{\text{LoS}}\) and \(\nu_{\text{NLoS}}\) denote the corresponding time of arrival (ToA) of the LoS and NLoS rays, \(N_{\text{clus}}\) and \(N_{\text{ray}}\) are the number of clusters and rays in the c-th cluster, \(\phi_Tx\) and \(\phi_{c,\ell}\) are the angles of departure/arrival (AoDs/AoAs) of the LoS and \(\ell\)-th ray c-th cluster NLoS, \(\nu_{\text{com}} = v/\lambda\) and \(\nu_{\text{NLoS},c,\ell}\) has the same expression as \(\alpha_{\text{Rx}}(\cdot)\) with the number of Rx antenna elements \(N_{\text{Rx}}\) instead.

Then, let us sketch the expressions of path gains and MP components. Firstly, similar to the sensing model in (9), the single-trip path loss of LoS is given by [28]

\[
\alpha_{\text{com}}(f_c, r) = \left( \frac{\lambda}{4\pi r} \right)^{2} e^{-\frac{1}{2} K(f_c) r} e^{-\frac{2\pi}{2} r}.
\]

(18)

Secondly, the ToA of NLoS rays consists of two parts, i.e., \(\tau_{\text{NLoS}} = T_{\text{NLoS}} + \tau_{\text{NLoS}}\), where \(T_{\text{NLoS}}\) and \(\tau_{\text{NLoS}}\) denote the cluster and ray within cluster ToAs, respectively, both of which follow exponential distributions conditioned on the arrival time of the previous cluster/ray, i.e., [36]

\[
p(T_{\text{c}}|T_{\text{c}-1}) = \Lambda e^{-\Lambda(t_{\text{NLoS}} - T_{\text{c}-1})}, \quad T_{\text{c}} > T_{\text{c}-1},
\]

(19)

\[
p(t_{\text{c}}, t_{\text{c}-1}) = \Lambda e^{-\Lambda(t_{\text{NLoS}} - T_{\text{c}-1})}, \quad t_{\text{c}} > t_{\text{NLoS}},
\]

(20)

where \(\Lambda\) and \(\hat{\Lambda}\) account for the cluster and ray arrival rates, respectively. Accordingly, the number of clusters \(N_{\text{clus}}\) and the number of rays within each cluster \(N_{\text{ray}}\) follow two independent Poisson distributions with rates \(\Lambda\) and \(\hat{\Lambda}\), respectively.

Consequently, the NLoS path loss and its mean-square gain are respectively expressed as [36]

\[
\alpha_{c,\ell} N_{\text{LoS}}(f_c, r) = |\alpha_{c,\ell} N_{\text{LoS}}(f_c, r)| e^{j\varphi_{c,\ell}},
\]

(21)

\[
E[|\alpha_{c,\ell} N_{\text{LoS}}(f_c, r)|^2] = |\alpha_{c,\ell} N_{\text{LoS}}(f_c, r)|^2 e^{\frac{j2\pi f_{\text{com}} N_{\text{LoS}}}{\nu_{\text{com}}}} e^{-\frac{\nu_{\text{com}}}{2} r},
\]

(22)

where \(\varphi_{c,\ell}\) is a phase shift with \(\varphi_{c,\ell} \sim \mathcal{U}(0, 2\pi)\), and (22) indicates that the average MP gain follows a double exponential decay profile with the cluster and ray decay factors (also called the power-decay time constants), \(\Gamma\) and \(\hat{\Gamma}\).

Last, for the convenience in our single-UE system, a 2D isotropic scattering environment is introduced, where the AoAs of the NLoS rays are uniformly distributed, and the Doppler spectrum follows the Flat model.

D. Sensing-Aided THz Communication Model

In accordance with the TDD framework proposed in Section II, after Period 1, the ISAC system will have the 3D parameters (i.e., range, velocity, and angle) estimation results and estimates of the DL communication channel (17) by employing least-squares (LS) estimator, denoted by \(H_{\text{com}}\). The ISAC system then transmits ISAC signal containing DL data via these prior information.

In this paper, we consider spatial multiplexing and fully digital precoding architecture in the communication case. Refer to (2), the precoded (DFT-s)-OFDM data grid of the l-th independent stream \(X_{l,\text{ISAC}}^{\text{TF}} \in \mathbb{C}^{N_{s} \times N_{\text{sym}}} \) can be given by

\[
X_{l}^{\text{TF}} = \begin{cases} [X_{l,0} \odot \mathbf{f}_{\text{com}}], & \text{for OFDM,} \\ \mathbf{F}_{N_{s}} [X_{l,0} \odot \mathbf{f}_{\text{com}}], & \text{for DFT-s-OFDM,} \end{cases}
\]

(23)

where \(l = 1, 2, \ldots, N_{s}\) with \(N_{s} = \min(N_{\text{ISAC}}, N_{\text{UE}})\) being the number of independent data streams, \([X_{l,0} \odot \mathbf{f}_{\text{com}}]\) denotes information symbols of the l-th stream with a \(M\)-ary quadrature amplitude modulation (QAM), and \(\mathbf{F}_{N_{s}}\) represents precoding weights (i.e., the transpose of the left singular matrix) per data stream based on channel diagonalization of \(H_{\text{com,l}} \in \mathbb{C}^{N_{c} \times N_{\text{sym}}} \) by using singular value decomposition (SVD).

Compared with (3), the baseband OFDM/DFT-s-OFDM communication signal of the l-th data stream after the digital precoding and Doppler pre-compensation can be written as

\[
s_{l}(t) = \frac{1}{\sqrt{N_{c}}} \sum_{m=0}^{N_{s}-1} \sum_{n=0}^{N_{\text{sym}}-1} [X_{l,\text{ISAC}}^{\text{TF}}]_{n,m} e^{j2\pi n\Delta f(t-mT_{\text{sym}})} e^{-j2\pi v_{\text{com}} t} \left( \frac{t - mT_{\text{sym}} + T_{\text{sym}}}{T_{\text{sym}}} \right),
\]

(24)

with \(v_{\text{com}} = v/\lambda\) being the value of Doppler compensation. Hence, the DL communication signal transmitted by the ISAC system in time domain is as follows

\[
s(t) = w(s(t))e^{j2\pi f_{\text{com}} t} \in \mathbb{C}^{N_{\text{ISAC}} \times 1},
\]

(25)

where \(s(t) = [s_{1}(t), \ldots, s_{N_{s}}(t)]^{T} \in \mathbb{C}^{N_{s} \times 1}\) stands for the total transmitted data streams, and \(w \in \mathbb{C}^{N_{\text{ISAC}} \times N_{s}}\) denotes the replication matrix over the Tx antennas employed.

Afterward, plugging the estimated azimuth angle \(\hat{\theta}\) into (17) to implement sensing-aided THz narrow beam alignment, and then applying the channel model to (25) yields the signal received by the UE

\[
y_{\text{com}}(t) = \int H_{\text{com}}(t, \tau) \tilde{s}(t - \tau) d\tau + n_{\text{com}}(t)
\]

\[
= \alpha_{\text{com}} e^{j2\pi f_{\text{com}} - \hat{\tau}_{\text{com}}} H_{\text{ISAC}}(\hat{\theta}) G_{\text{ISAC}}^{\text{TF}}(\hat{\theta} - \pi) a_{\text{Rx}}(\hat{\theta} - \pi) \cdot a_{\text{ISAC}}^{\text{CT}(\hat{\theta})} \tilde{s}(t - \tau)_{\text{com}}
\]

\[
\cdot \sum_{c=1}^{N_{\text{clus}}} \sum_{\ell=1}^{N_{s}} \alpha_{c,\ell} N_{\text{LoS}}(\tau - \tau_{\text{LoS}}) e^{j2\pi f_{\text{com}} \tau} G_{\text{ISAC}}(\phi_{c,\ell}) G_{\text{ISAC}}^{\text{TF}}(\phi_{c,\ell}) a_{\text{Rx}}(\phi_{c,\ell})
\]

\[
\cdot a_{\text{ISAC}}^{\text{CT}(\phi_{c,\ell})} \tilde{s}(t - \tau_{\text{LoS}}) + n_{\text{com}}(t),
\]

(26)

where \(n_{\text{com}}(t) \in \mathbb{C}^{N_{\text{Rx}} \times 1}\) is the additive noise at the receiver of the UE with the total power of \(\sigma_{\text{RF}}^{2} = k_{B} T_{\text{sys}} B N_{\text{fig}},\) with \(N_{\text{fig}}\) denoting the UE’s Rx noise figure.
IV. WAVEFORM NUMEROLOGY DESIGN FOR THZ ISAC

In this section, to design a flexible and reconfigurable frame structure to balance communication and sensing performance and adapt to different applications, constraints on ISAC waveform numerology design are listed first. Based on these limitations, trade-offs among performance indicators are discussed subsequently. Eventually, in view of the trade-offs, we combine the sensing and communication performance parameters with scenario demands to formulate general guidelines for OFDM/DFT-s-OFDM frame structure design.

A. Waveform Numerology Design Constraints

1) Communication Channel Characteristics Constraints: To avoid inter-symbol interference (ISI), the CP length should be chosen larger than the maximum excess delay of the channel $\tau_c$ [37], i.e., $T_{\text{CP}} \geq \tau_c$. In addition, to expect flat-fading channels and avoid ICI, the subcarrier spacing must be chosen larger than the maximum Doppler spread and also smaller than the coherence bandwidth [37], i.e., $f_{\text{D,max}} = \Delta f < B_c$, with $f_{\text{D,max}} = \nu_{\max}/\lambda$ being the maximum Doppler spread in the communication case, $B_c = 1/\Delta\tau$, the coherence bandwidth [14] and $\tau_{\text{MS}}$ the root mean square (RMS) delay spread. On the other hand, the OFDM symbol duration is typically designed to be much larger than the delay spread and also much less than the coherence time, i.e., $\tau_{\text{MS}} \approx T_u \ll T_c$, where $T_u = \frac{2\nu_0}{f_{\text{D,max}}} \frac{f_{\text{max}}}{f_{\text{D,max}}}$. The coherence time [14].

2) PAPR Constraints: As an inherent problem, the high PAPR of OFDM/DFT-s-OFDM baseband signals with $L$ times oversampling is defined as

$$\text{PAPR} = \frac{\max_{0 \leq n \leq L-1} |s[n]|^2}{\mathbb{E}[|s[n]|^2]}.$$  \hfill (27)

Existing works have shown that OFDM signals with larger number of subcarriers usually have higher PAPRs [38]. Hence, choosing a smaller number of subcarriers within the desirable range is crucial to minimize the PAPR.

3) Sensing Requirements Constraints: For 3D-FFT algorithm, it is necessary to avoid the ambiguous estimation. The maximum unambiguous range is limited by the effective symbol duration, i.e., $r_{\text{max.unamb}} = \frac{c\tau_c}{2}$. Meanwhile, to preserve orthogonality in time domain, the maximum tolerable range is limited by the CP duration [39], i.e., $r_{\text{max.toler}} = \frac{c\tau_{\text{CP}}}{2}$. On the frequency domain side, likewise, in order to ensure the orthogonality of the subcarriers, the subcarrier spacing must be chosen to $\Delta f \geq \frac{1}{f_{\text{D,max}}}$, with $f_{\text{D,max}} = 2\nu_{\max}/\lambda$, resulting in the maximum tolerable relative radial velocity given by $v_{\text{max.toler}} = \frac{c}{\Delta f}$ [39]. Differently, the maximum unambiguous relative radial velocity is reduced by $\nu_{\text{ISAC}}$ in the TDM case [24], i.e., $v_{\text{max.unamb}} = \frac{c}{4f_{\text{ISAC}}} \frac{\nu_{\text{sym}}}{}$. The maximum unambiguous relative radial velocity is given by $\nu_{\text{ISAC}}$. In Fig. 2(a), the maximum tolerable range increases when $N_c$ increases. In Fig. 2(b), the maximum sensing range increases when $N_c$ increases, while the maximum sensing velocity is the opposite. Meanwhile, the maximum sensing range and velocity change inversely with the increase of $\alpha$. Last but not least, increasing $N_c$ and $\alpha$ also affects the data rate (Fig. 2(c)), as it changes the number of synchronization symbols $R_{\text{sym}}$ and the CP length respectively, which in turn has a negative effect on the data rate. Thus, appropriate choices for $N_c$ and $\alpha$ are the keys to maximize the effective symbol rate (i.e., UE experienced rate), which is given by

$$\text{SNR}_{\text{sen}}(r) = \frac{P_{\text{ISAC}} G_{\text{ISAC}}|G_{\text{Rx}}|}{\sigma_{\text{sen}}^2} |\alpha_{\text{ISAC}}(f_c, r)|^2.$$  \hfill (30)

After virtual array processing at the receiver of the ISAC systems, the coherent accumulation of 3D-FFT algorithm increases the sensing SNR by factor $N_c N_{\text{sym}} N_{\text{vrit}}$ [44], results in the SNR of the periodogram expressed by $\text{SNR}_{\text{p}} = \text{SNR}_{\text{sen}} |G_p|$, where $G_p = N_c N_{\text{sym}} N_{\text{vrit}}$ is the total processing gain. We employ the 2D-constant false alarm rate (CFAR) method to identify the single UE in the presence of background noise, and the minimum SNR required with the probability of false alarm $P_{\text{fa}}$ is $\text{SNR}_{\text{sen.min}} = -\ln(1 - \frac{\gamma}{T - P_{\text{fa}}})$ [37].

B. Trade-offs in Waveform Numerology Design

The main numerologies of OFDM/DFT-s-OFDM waveforms for flexible design are the bandwidth $B$, the number of subcarriers $N_c$, the subcarrier spacing $\Delta f$, the number of symbols $N_{\text{sym}}$, and the CP rate $\alpha$. In practical 6G services, available bandwidth resources are usually given first, in which case $\Delta f$ changes with $N_c$. Thus, we mainly focus on $N_c$ and $\alpha$ for trade-offs in waveform numerology design.

For fixed bandwidth, trade-offs between the sensing and communication performance are shown in Fig. 2. As shown in Fig. 2(a), the PAPR increases and the range PLSR decreases with $N_c$ increasing. In Fig. 2(b), the maximum sensing range increases when $N_c$ increases, while the maximum sensing velocity is the opposite. Meanwhile, the maximum sensing range and velocity change inversely with the increase of $\alpha$. Last but not least, increasing $N_c$ and $\alpha$ also affects the data rate (Fig. 2(c)), as it changes the number of synchronization symbols $R_{\text{sym}}$ and the CP length respectively, which in turn has a negative effect on the data rate. Thus, appropriate choices for $N_c$ and $\alpha$ are the keys to maximize the effective symbol rate (i.e., UE experienced rate), which is given by

$$\chi(\tau, \nu, \theta) = \left| a_{\text{Rx}}^{\text{ISAC}}(\theta) R(\tau, \nu) a_{\text{Tx}}^{\text{ISAC}}(\theta) \right|^2 + \left| a_{\text{Rx}}^{\text{ISAC}}(\theta) a_{\text{Rx}}^{\text{ISAC}}(\theta) \right|^2,$$  \hfill (28)
\[ \mathcal{R} = (N_{\text{sym}} - n_{\text{sym}})N_c/T_c, \text{ with } n_{\text{sym}} \text{ being approximated by } n_{\text{sym}} = T_I/T_c. \]

As we have explored above, there are three trade-offs among these communication and sensing performance metrics, i.e., high PAPR versus low range PSLR, large sensing range versus low sensing velocity, and high effective data rate versus short sensing range. Following, we will develop waveform frame structure design guidelines based on these trade-offs.

### C. Frame Structure Design Guidelines

The simplest requirement is range resolution, since it only relates to the bandwidth size, which means that the bandwidth needed can be chosen first, that is, \( B \geq \frac{c_0}{r_{\text{req}}} \). Once \( B \) is determined, and remaining required parameters are provided by the practical systems, we regard the effective symbol rate maximization as a single-objective optimization by considering both communication and sensing requirements as constraints.

Specifically, after simplifying and combining the conditions in Section IV-A, the frame structure design guidelines for (DFT-s-)OFDM-based ISAC waveforms are formulated as

\[
\arg \max_{N_c, \alpha, N_{\text{sym}}} \mathcal{R} = \frac{B}{1 + \alpha} - \frac{N_c}{T_c}
\]

\[
\text{s.t. } C1 : T_{\text{CP}} > \tau_e
\]

\[
C2 : 10f_{\text{D,max}} \leq \Delta f \ll B_c
\]

\[
C3 : T_{\text{CP}} \geq \frac{2r_{\text{req}}}{c_0}
\]

\[
C4 : \frac{c_0}{2f_cN_{\text{sym}}T_{\text{sym}}} \leq \Delta v_{\text{req}}
\]

\[
C5 : \min \left( \frac{c_0\Delta f}{20f_c}, \frac{c_0}{4f_cN_{\text{sym}}T_{\text{sym}}} \right) \geq v_{\text{req}}
\]

\[
C6 : \text{PSLR}_{r}(N_c) \leq \text{PSLR}_{r,\text{th}}
\]

\[
C7 : \text{SNR}_{\text{sen}}(r_{\text{req}})N_cN_{\text{sym}}N_{\text{virt}} \geq \text{SNR}_{\text{sen,min}}
\]

\[
C8 : N_c = 2^k, N_{\text{sym}} = 2^{k_2}, k_1, k_2 \in \mathbb{N}_+
\]

\[
C9 : \alpha \in \{1/4, 1/8, 1/16, 1/32\}
\]

where \( r_{\text{req}}, \Delta v_{\text{req}}, v_{\text{req}} \) are, respectively, the requirement of sensing range, velocity resolution, and sensing velocity for different applications, \( \text{PSLR}_{r,\text{th}} \) is the threshold of the range PSLR, and \( \mathbb{N}_+ \) denotes the positive integer domain.

In (31), the first and the second constraints are communication constraints that aim at preventing DL transmissions with ISI, ICI, and non-flat fading. Constraints C3 to C7 represent sensing constraints to adapt to support use cases with diverse requirements for 6G ISAC. Last but not least, for convenience, C8 and C9 denote numerology specifications, following OFDM standard definitions in [45].

### V. Link-Level Simulator for THz MIMO ISAC Systems

To evaluate the sensing and communication performance of the waveforms derived from the proposed design guidelines, we develop a link-level simulator for THz MIMO ISAC systems based on the ISAC framework in Section II and the system model in Section III. In this section, the overall architecture and visualized UI of the simulator are demonstrated.

#### A. Simulator Architecture

The proposed simulator supports very flexible and elaborate parameters configuration and integrates link-level signal processing in the sensing and communication case. Herein, the main function modules, classified into four categories in Fig. 3(a), are stated first. Subsequently, the corresponding signal processing flow is shown in Fig. 3(b).

1) Parameters Initialization: This module aims to configure all initial parameters for other function modules before running the simulation. Concretely, it consists of five types of parameters: ISAC system parameters, UE parameters, waveform parameters, THz channel parameters, and 2D-CFAR parameters. In order to facilitate user customization, all parameters are contained in a struct variable that can be easily invoked by other functions. However, the ranges of values for these parameters are restricted to circumvent abnormal configurations.

Detailedly, ISAC system parameters are composed of mobility settings, including its 2D position \( \mathbf{p}_{\text{ISAC}} = [x, y]^T \), 2D absolute velocity \( \mathbf{v}_{\text{ISAC}} = [x, y]^T \), and antenna parameters. Likewise, UE parameters are composed of mobility settings (including the mobile range from the UE to the ISAC system \( r \), 2D absolute velocity \( \mathbf{v}_{\text{UE}} = [x, y]^T \), and azimuth angle \( \theta \), ULA configurations at the UE, and target settings (containing target statistical model and mean
RCS $\sigma_{RCS}$). Waveform parameters refer to the physical layer configurations made up of OFDM/DFT-s-OFDM numerologies, carrier frequency $f_c$, modulation order $M$, channel coding type, code rate $\eta$, and channel equalization method. **THz channel parameters** is composed of molecular absorption coefficient parameters which are directly retrieved from the high-resolution transmission molecular absorption (HITRAN) database [46] and MP parameters. Note that the THz channel of farther apart Tx-Rx pair generally consists of fewer clusters [47], especially in outdoor scenarios, where the average number of clusters is only around 3 [30], [48]. To this end, the simulator sets an upper bound of the number of clusters $N_{\text{clus}, \text{max}}$. As a result, the number of clusters generated by the simulator can be expressed as $N_{\text{clus}} = \min(N_{\text{clus}, \text{max}}, N_{\text{clus}})$, where $N_{\text{clus}}$ follows the stochastic model in Section III-C.

2D-CFAR parameters contain basic detection parameters, including CFAR type, false alarm rate $P_{fa}$, and the number of rows and columns of the guard/training band cells $N_{\text{guard}} = [N_{\text{row, guard}}, N_{\text{col, guard}}]$, $N_{\text{train}} = [N_{\text{row, train}}, N_{\text{col, train}}]$. 

2) Sensing Link-level Simulation: We aim to achieve the echo sensing function in this module, corresponding to the sensing processing part of Period 1 in Fig. 3(b). Specifically, motion management module first generates the position and mobility of the ISAC system and UE. Next, in the Tx signal generation, DL preamble signals under TDM-MIMO coding are generated, amplified at the front-end and transmitted through the antennas. After applying the channel generated by the sensing channel generation, as Fig. 3(b) shows, the received signals will undergo demodulation, preamble symbol extraction, TDM decoding, 3D-FFT algorithm, and 2D-CFAR detection in the Rx signal processing. Besides, our simulator applies Hanning window functions to the input data cube before performing FFT operations for the efficient decrease of sidelobe levels, which is capable of improving detection reliability. In the end, estimates storage stores the estimates of range/velocity/angle in the workspace for subsequent communication simulations.

3) Communication Link-level Simulation: This module aims to achieve the sensing-aided communication function, as Fig. 3(b) shows, corresponding to the entire Period 2 and the part of communication processing in Period 1. In addition, the simulator implements convolutional channel coding and soft-decision demodulation to further improve communication reliability with a low computational cost.
Specifically, in the *DL transmission preparation*, pre-amplification, timing recovery, OFDM/DFT-s-OFDM demodulation, frequency domain channel estimation based on LS method, and calculation of the feedback weights based on SVD method are performed first, and then the estimation results are read from the workspace for Doppler pre-compensation and THz beam alignment enhancement. *Tx signal generation* includes channel coding, QAM modulation with Gray mapping, splitting of individual data stream to multiple transmit streams, fully-digital precoding based on feedback weights, OFDM/DFT-s-OFDM modulation, and front-end processing. However, not all subcarriers are used to carry data in practical systems, so the simulator allocates a fixed number of subcarriers as direct current (DC), pilot, and guard-band subcarriers. Among them, the DC subcarrier served as buffers between symbols locates at the center of the frequency band, while the guard-band subcarriers provide buffers between adjacent-band signals to reduce interference caused by spectral leakage. After propagating through the THz channel generated by the *communication channel generation*, the original information embedded in the DL data signal is ultimately recovered at the UE, when *Rx signal processing* contains front-end amplification and synchronization, OFDM/DFT-s-OFDM demodulation, channel equalization based on zero-forcing (ZF) or minimum mean square error (MMSE) method, soft-decision demodulation based on approximate log-likelihood ratio (LLR) algorithm, and decoding.

4) **Visualization:** As a link-level simulator, it can not only exhibit specific display functions, including RV/RA images, 2D-CFAR detection results, Tx/Rx constellation, and channel response pattern, but also support waveform evaluation of key performance indicators, such as, PAPR, spectral efficiency (SE), effective data rate, bit error rate (BER), and error vector magnitude (EVM).

### B. Visualized User Interface

Moreover, compared with the existing advanced simulators, we provide a fully visualized and interactive UI (Fig. 4) for intuitive operation. Consistent with the aforementioned modules, the parameters setting of the simulator is located at the top of the UI, most of which can be self-defined by the user via keyboard, while some of which can only be selected via the drop-down menu that are illustrated as follows:

- Waveform type: OFDM or DFT-s-OFDM.
- Modulation order: 4, 16, 64, or 256, i.e., square QAM.
- Number of subcarriers: 128, 256, ..., or 8192.
- Number of symbols: 16, 32, ..., or 8192.
- CP rate: 1/32, 1/16, 1/8, or 1/4.
- Channel coding type: None or convolutional.
- Code rate: Common values with 1/3, 1/2, 2/3, 3/4, 5/6, or 7/8, and 1 corresponding to without channel coding.
- Channel equalization method: ZF or MMSE.
- CFAR type: Cell-averaging (CA), greatest of CA (GOCA), or smallest of CA (SOCA).
- Number of Tx/Rx antennas: 2, 4, ..., or 64.
- Target statistical model: Nonfluctuating or Swerling.

After selecting the parameters in the interface and running the simulation, as Fig. 4 shows, RV/RA/2D-CFAR images, Tx/Rx constellation, and delay-domain channel response of NLoS are displayed as pictures, while range/velocity/angle estimates and communication performance indicators are shown in the text box at the bottom of the UI, respectively.

### VI. URBAN V2V APPLICATION CASE

In this section, we take the urban V2V application case as an example, waveform numerologies are obtained first by adopting the proposed frame structure design guidelines with expected requirements, and then its simulation results are presented to verify the capabilities of the simulator by a fair comparison of OFDM and DFT-s-OFDM waveforms.

#### A. System Parameters Configuration

For typical mid-range V2V applications in the urban grid scenario, introduced by 3GPP TR 37.885 [49], a maximum range of 50 m with a resolution of up to 0.2 m, a maximum relative radial velocity of 60 km/h with a resolution of up to 0.2 m/s [39], and a angular resolution of 4° [50] are expected.
Combined with the measurements of urban V2V THz channel in [29], communication constraints and sensing requirements for the waveform design are summarized in Table II.

Abiding by IEEE Std. 802.15.3d [51], we design the THz MIMO ISAC systems to operate in the 252 GHz band, and a supported channel bandwidth of 2.16 GHz is chosen to meet the range resolution requirement first. Then, based on the common parameters of automobiles given by [52] in Table III and requirements for urban V2V cases in Table II, OFDM/DFT-s-OFDM waveform numerologies can be obtained by employing the frame structure design guidelines proposed in Section IV-C, eventually merged to show in Table III.

**B. Sensing Performance Evaluation**

With parameters from Table III, the considered ISAC vehicle equipped with 4Tx-8Rx sparse ULAs theoretically attains a maximum sensing range of 71.06 m with a resolution of 0.07 m, a maximum sensing velocity of ±31.37 m/s with a resolution of 0.12 m/s, and an angular resolution of 3.58°, which perfectly cover the sensing requirements in Table II. By means of the presented simulator, we simulate a practical urban V2V scenario, where an ISAC vehicle and a UE vehicle in adjacent lanes travel in the same direction. Scenario parameters are listed in Table IV, resulting in a initial relative radial velocity of approximately 14.1 m/s.

Fig. 5 shows the WAFs from the profile perspective. In Fig. 5(a), depending on the width of the main peak, the range PSLR of OFDM and DFT-s-OFDM is about −31.9 dB and −26.8 dB, respectively, and both are below the threshold in Table II to prevent the masking effect. Notice that the DFT-s-OFDM waveform has a higher sidelobe level than OFDM, due to the fact that the benefits of DFT-s-OFDM in terms of reduced PAPR values come at the expense of reduced range PSLR performance. In Fig. 5(b), two waveforms with one symbol both suffer a velocity ambiguity of about 235 m/s and a velocity PSLR of −13.2 dB, while 2048 symbols in Table III are desired to make velocity resolution approach to 0.12 m/s described in the preceding paragraph. From the spatial perspective, the two-way beam pattern of virtual arrays in Fig. 5(c) shows a narrower beamwidth and a four-times improved angular resolution with the same antenna resources.

The plots of the normalized sensing images in RV and RA domains are depicted in Fig. 6. It is clear that the target vehicle is accurately located in the three dimensions of range, relative radial velocity, and azimuth angle whilst the imaging performance of OFDM and DFT-s-OFDM is almost identical. Meanwhile, with the help of Hanning windows, high sidelobes in velocity and angle domains are effectively eliminated, while there is still a certain level of sidelobe in range domain because of the range migration effect in wideband systems.

In order to further evaluate the estimation performance, the sensing accuracy comparison of the target range, velocity, and angle estimation is provided and compared with root Crámer-Rao lower bound (CRLB). According to fundamental limits of colocated MIMO radar for single-target sensing given by [53] and the derivation of the virtual array case in [44], the CRLBs for the variances of range, velocity, and angle estimates for OFDM/DFT-s-OFDM are written by

\[
\text{CRLB}_r = \frac{3\pi^2}{8\pi^3 T_2 c^2 N_{\text{center}}^2 N_{\text{sym}}^2 (N_c^2 - 1) \text{SNR}_{\text{sen}}}, \\
\text{CRLB}_v = \frac{3\pi^4}{8\pi^3 T_2 c^2 N_{\text{center}}^2 N_{\text{sym}}^2 (N_c^2 - 1) \text{SNR}_{\text{sen}}}, \\
\text{CRLB}_\theta = \frac{\pi^2 \cos^2(\theta) N_{\text{center}}^2 N_{\text{sym}}^2 (N_c^2 - 1) \text{SNR}_{\text{sen}}}{6},
\]

where SNR_{sen} corresponds to (30). The root mean square errors (RMSEs) of the estimations are illustrated in Fig. 7(a), 7(b), and 7(c). Both OFDM and DFT-s-OFDM waveforms are capable of achieving the same estimation error of the UE vehicle’s range, relative radial velocity, and azimuth angle, obtained as 0.07 m, 0.004 m/s, and 1.79° over −43 dB sensing SNRs, which indicates that the ISAC vehicle with parameters in Table III is able to achieve millimeter-level, millimeter per second-level, and sub-degree-level sensing accuracy of range, velocity, and angle at low SNRs in this simulated scenario.

---

**TABLE II**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum excess delay $\tau_e$</td>
<td>200 ns</td>
</tr>
<tr>
<td>LoS/NLoS RMS delay spread $\tau_{\text{Emis}}$</td>
<td>25.7/12.9 ns</td>
</tr>
<tr>
<td>LoS/NLoS coherence bandwidth $B_c$</td>
<td>7.8/15.5 MHz</td>
</tr>
<tr>
<td>Maximum range requirement $r_{\text{req}}$</td>
<td>50 m</td>
</tr>
<tr>
<td>Range resolution requirement $\Delta r_{\text{req}}$</td>
<td>0.2 m</td>
</tr>
<tr>
<td>Maximum relative radial velocity requirement $v_{\text{req}}$</td>
<td>16.7 m/s</td>
</tr>
<tr>
<td>Velocity resolution requirement $\Delta v_{\text{req}}$</td>
<td>0.2 m/s</td>
</tr>
<tr>
<td>Angular resolution requirement $\Delta \theta_{\text{req}}$</td>
<td>$4^\circ$</td>
</tr>
<tr>
<td>Range PSLR threshold $\text{PSLR}_{\text{r,th}}$</td>
<td>$-20$ dB</td>
</tr>
</tbody>
</table>

---

**Fig. 5.** Comparison of wideband ambiguity functions for the considered THz MIMO ISAC systems based on OFDM and DFT-s-OFDM with one symbol.
respectively. However, as is observed from all three figures, the OFDM waveform significantly reduces the estimation error by about 12 dB by contrast with the DFT-s-OFDM waveform, caused by the single-carrier characteristic of DFT-s-OFDM that reduces the equivalent sensing processing gain, just similar to its negative effect on the performance of range PSLR.

C. Communication Performance Evaluation

On the communication side, in line with the simulator construction details in Section V-A, a fraction of 4096 subcarriers in Table III is assigned as pilots and null subcarriers. Herein, Table V shows the adopted parameters in the DL communication case, in which the THz channel parameters derive from [14]. First, as an basic indicator of achievable rate, the two waveforms perform the same SE of $\frac{N_{\text{data}}}{2} \log_2 M = 2.8$ bit/s/Hz without additional loss in the DFT-s-OFDM case due to the employment of one spreading factor-based localized subcarrier mapping in (1) and (23), ultimately resulting in high-rate data transmission experienced by the UE vehicle calculated by $R = (1/T_{\text{sym}} - 1/T_c) N_c N_{\text{data}} \eta \log_2 M$ of about 22.56 Gbps, which sufficiently enables large-capacity real-time transmission of data and images in 6G V2V.

Next, in Fig. 8, we implement four-times oversampling to precisely evaluate the baseband PAPR of the OFDM and DFT-s-OFDM waveforms by considering statistical results regarding the complementary cumulative distribution function (CCDF). It is learnt that DFT-s-OFDM has lower PAPR than OFDM, in particular, the PAPR values of DFT-s-OFDM are approximately 3 dB lower than OFDM at the CCDF of 10^{-4}, by which we can decrease the nonlinear distortion of power amplifiers with lower power backoff and further significantly improve the energy efficiency in the THz ISAC systems.

Finally, we compare the BER performance of the OFDM and DFT-s-OFDM waveforms with and without sensing assistance and channel coding. As Fig. 9 shows, sensing-aided Doppler compensation greatly mitigates the severe damage to subcarrier orthogonality caused by the ultra-high Doppler spread in the THz band. Furthermore, $10^{-8}$ BER level is achieved at communication SNR of about 25 dB for both waveforms thanks to the great gain generated by channel coding and soft demodulation. However, this advantage comes at the price of more computation and lower data rate.

Table III

<table>
<thead>
<tr>
<th>System parameters</th>
<th>Values</th>
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</thead>
<tbody>
<tr>
<td>Carrier frequency $f_c$</td>
<td>252 GHz</td>
</tr>
<tr>
<td>Bandwidth $B$</td>
<td>2.16 GHz</td>
</tr>
<tr>
<td>Number of subcarriers $N_c$</td>
<td>4096</td>
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<tr>
<td>Number of symbols $N_{\text{sym}}$</td>
<td>2048</td>
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<tr>
<td>CP rate $\alpha$</td>
<td>1/4</td>
</tr>
<tr>
<td>Target statistical model</td>
<td>Swerling I</td>
</tr>
<tr>
<td>Mean RCS $\sigma_{\text{RCS}}$</td>
<td>20 dBsm</td>
</tr>
<tr>
<td>Path loss exponent $n_c$</td>
<td>2</td>
</tr>
<tr>
<td>Absorption coefficient $K$</td>
<td>0.00037 m^{-1}</td>
</tr>
</tbody>
</table>

Table IV

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position of the ISAC vehicle $\mathbf{p}_{\text{ISAC}}$</td>
<td>[0, 0]^T</td>
</tr>
<tr>
<td>Velocity of the ISAC vehicle $\mathbf{v}_{\text{ISAC}}$</td>
<td>30 m/s</td>
</tr>
<tr>
<td>Velocity of the UE vehicle $\mathbf{v}_{\text{UE}}$</td>
<td>20^\circ</td>
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<tr>
<td>Azimuth angle $\theta$</td>
<td></td>
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</table>

Table V

<table>
<thead>
<tr>
<th>Parameters</th>
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<tbody>
<tr>
<td>Number of pilot subcarriers $N_{\text{pilot}}^\text{max}$</td>
<td>8</td>
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<tr>
<td>Number of guard-band subcarriers $N_{\text{guard}}^\text{max}$</td>
<td>13</td>
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<td>Number of DC subcarriers $N_c^\text{DC}$</td>
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<tr>
<td>Number of data subcarriers $N_{\text{data}}^\text{max}$</td>
<td>4074</td>
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<td>QAM modulation order $M$</td>
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<tr>
<td>Convolutional channel code rate $\eta$</td>
<td>7/8</td>
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<tr>
<td>Maximum number of clusters $N_{\text{clu, max}}^\text{max}$</td>
<td>3</td>
</tr>
<tr>
<td>Cluster, ray arrival rate $A$, $A$</td>
<td>0.13, 0.37 ns^{-1}</td>
</tr>
<tr>
<td>Cluster, ray decay factor $\Gamma$, $\Gamma$</td>
<td>3.12, 0.91 ns</td>
</tr>
</tbody>
</table>
Velocity estimation performance.

Angle estimation performance.

<table>
<thead>
<tr>
<th>Velocity RMSE (m/s)</th>
<th>Angle RMSE (°)</th>
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<tbody>
<tr>
<td>10</td>
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CCDF

BER

VII. CONCLUSION

To catalyze the standardization and industrialization of THz MIMO ISAC technologies for 6G networks, a comprehensive link-level simulator with a UI supporting detailed configuration and visualization is proposed. In particular, the simulator integrates virtual array-based 3D estimation with sensing-aided multi-stream transmission through the novel TDD framework. It also captures the typical peculiarities of THz channels, including wideband echo, molecular absorption, and cluster-based propagation. General design guideline for OFDM and DFT-s-OFDM numerologies is presented for parameter initialization. At the end, a typical urban V2V scenario is conducted via 2D movements simulation to demonstrate the capabilities of the simulator. Furthermore, the proposed simulator can be employed for design and analysis of the THz ISAC systems.

Looking to the future work, we plan to introduce more advanced waveforms, such as orthogonal time frequency space (OTFS) and DFT-s-OTFS. In addition, the extension to multi-user sensing and communication is also achievable to make the simulator applicable for more services in 6G.

REFERENCES
