SAND2019-1728C

Sandia National Laboratories

An Isofrequency Remapping Scheme for Harmonic Balance Methods

Andy Huang*, Xujiao Gao*, Lawrence Musson*, Gary Hennigan*, Mihai Negoita*
ahuang@sandia.gov, xngao@sandia.gov, lcmusso@sandia.gov, glhenni@sandia.gov, mnegoit@sandia.gov
* Electrical Sciences and Modelling organization, Sandia National Laboratories, Albuquerque, NM

SIAM Computational Science and Engineering (CSE) Feb. 25 - Mar. 1, 2019

Objective

Harmonic balance methods are applied to solve parabolic partial differential equations in the frequency domain when periodic boundary conditions are applied.

Frequency remapping schemes enhance the efficiency of the harmonic balance method. However, **existing remapping methods overlook degenerate frequencies, resulting in incorrect numerical reformulations**.

We designed an isofrequency remapping scheme to solve the problem introduced by degenerate frequencies, maintaining harmonic balance accuracy and efficiency.

Harmonic Balance Method

We briefly describe the harmonic balance method as it has recently been incorporated in **Charon** [1] for semiconductor physics modeling. Its implementation simultaneously supports multiple spatial discterization formulations.

For the electron drift-diffusion equation

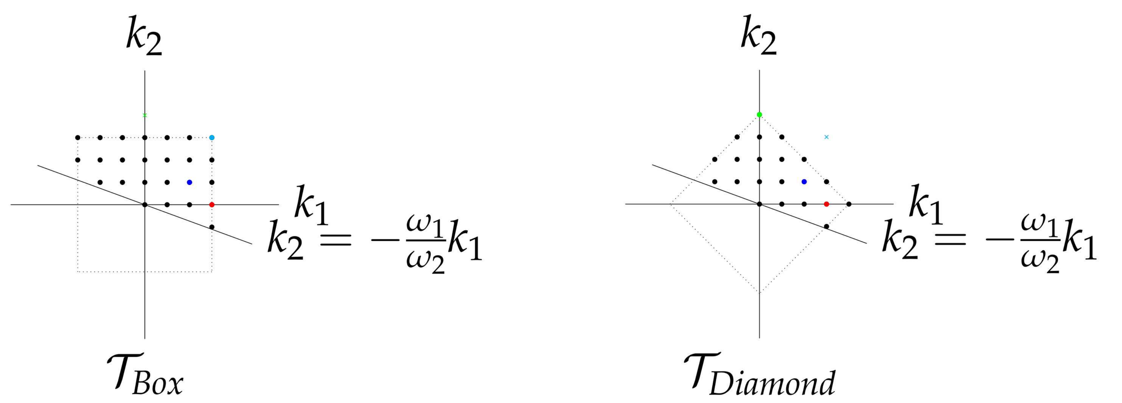
$$\frac{\partial n}{\partial t} + \mathcal{F}_n(n, p, \phi) = 0, \qquad (1)$$

a solution ansatz for $n(x, t)$ is introduced:

$$N_0(x) + \sum_{\vec{\alpha} \in \mathcal{T}} \left[N^c_{\vec{\alpha}}(x) \cos(2\pi\vec{\alpha} \cdot \vec{\omega}t) + N^s_{\vec{\alpha}}(x) \sin(2\pi\vec{\alpha} \cdot \vec{\omega}t) \right]. \qquad (2)$$

The **fundamental frequencies** $(\omega_1, \cdots, \omega_\ell) =: \vec{\omega} \in \mathbb{R}^\ell$ are boundary condition frequencies (wlog, $\omega_i < \omega_{i+1}$) and $\vec{\alpha} \in \mathbb{Z}^\ell$ produce fundamental frequency combinations $\vec{\alpha} \cdot \vec{\omega}$.

A **truncation scheme** $\mathcal{T}$ like the box or diamond scheme limits the harmonics appearing in the ansatz expression [2]. Note: we only require $\vec{\alpha} \in \mathcal{T}$ or $-\vec{\alpha} \in \mathcal{T}$.



The **harmonic balance equations** are the spatial residuals' Fourier coefficients. Balancing the $\cos(2\pi\vec{\alpha} \cdot \vec{\omega}t)$ coefficients of (1) for spatial element V and basis function $\Lambda(x)$ yields:

$$\begin{aligned} 0 =& \pi\vec{\alpha} \cdot \vec{\omega} \int_V N^s_{\vec{\alpha}}(\vec{x})\Lambda(\vec{x})\, d\vec{x} \\ &+ \sum_{m=0}^{L} w^m_{\vec{\alpha}} \mathcal{R}^\Lambda_n(n(t_m), p(t_m), \phi(t_m)) \end{aligned} \qquad (3)$$

where $w^m_{\vec{\alpha}}$ are quadrature weights determined by the Discrete Fourier Transform and $\mathcal{R}^\Lambda_n$ is a spatial residual. Note: L is a number of time sample points at least $2 \cdot |\vec{\omega}|_\infty$ to ensure accuracy by the Nyquist Sampling Theorem.

Frequency Remapping Method and Degenerate Frequencies

The Discrete Fourier Transform in (3) is prohibitively expensive for problems concerning many and/or great fundamental frequencies, i.e., when ℓ or $|\vec{\omega}|_\infty$ are large.

In the literature, **frequency remapping methods** like Artificial Frequency Mapping (AFM) [3] and Almost Periodic Fourier Transform (APFT) address this by performing a remapping $\vec{\omega} \mapsto \vec{\eta}$ in (2) and (3) to result in fewer summands for the Discrete Fourier Transform.

However, even in a two-tone simulation, for example, with

$$(\omega_1, \omega_2) = (1.0 \text{ MHz}, 1.1 \text{ MHz}),$$

the first fundamental frequency can be a **degenerate frequency** because two linear combinations coincide:

$$(10, 0) \cdot (\omega_1, \omega_2) = (-1, 10) \cdot (\omega_1, \omega_2)$$

If ω_1, ω_2 are remapped to η_1, η_2, we must maintain

$$(10, 0) \cdot (\eta_1, \eta_2) = (-1, 10) \cdot (\eta_1, \eta_2).$$

AFM and APFT do *not* account for degenerate frequencies.

Hence, if coefficients $\vec{\alpha}, \vec{\beta} \in \mathcal{T}$ yield $\vec{\alpha} \cdot \vec{\omega} = \vec{\beta} \cdot \vec{\omega}$, then an accurate remapping must yield $\vec{\alpha} \cdot \vec{\eta} = \vec{\beta} \cdot \vec{\eta}$. Furthermore, if $\vec{\alpha} \cdot \vec{\omega} \neq \vec{\beta} \cdot \vec{\omega}$, then we must also have $\vec{\alpha} \cdot \vec{\eta} \neq \vec{\beta} \cdot \vec{\eta}$. [4]

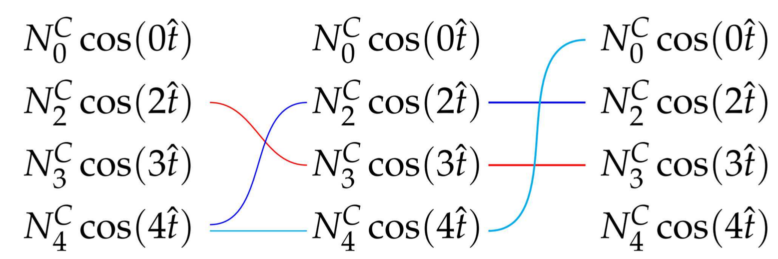
As the number of frequencies increases, more frequencies can degenerate (elements of $\mathcal{T} \cdot \vec{\omega}$ collide). For example,

$$\vec{\omega} = (2Hz, 3Hz, 4Hz)$$

has many combinations which produce $8Hz$ from non-linear terms; in particular, $n(t)^3$ produces

$$\left[\sum_{\vec{\alpha} \in \mathcal{T}} N^C_{\vec{\alpha}} cos(2\pi\vec{\alpha} \cdot \vec{\omega}t) + N^S_{\vec{\alpha}} sin(2\pi\vec{\alpha} \cdot \vec{\omega}t) \right]^3$$

which we expand visually (introducing $\hat{t} := 2\pi t$):



It is easy to see that there are collisions:

$$\begin{aligned} \cos(2\hat{t})\cos(3\hat{t})\cos(3\hat{t}) &= N_2N_3N_3 \cos((1,2,0) \cdot \vec{\omega}) + \cdots \\ \cos(4\hat{t})\cos(2\hat{t})\cos(2\hat{t}) &= N_4N_2N_2 \cos((2,0,1) \cdot \vec{\omega}) + \cdots \\ \cos(4\hat{t})\cos(4\hat{t})\cos(0\hat{t}) &= N_4N_4N_0 \cos((0,0,2) \cdot \vec{\omega}) + \cdots \end{aligned}$$

where the three truncation coefficients

$$\vec{\alpha} := (1, 2, 0), \quad \vec{\beta} := (2, 0, 1), \quad \vec{\gamma} := (0, 0, 2)$$

all yield $\vec{\alpha} \cdot \vec{\omega} = \vec{\beta} \cdot \vec{\omega} = \vec{\gamma} \cdot \vec{\omega} = 8Hz$.

Isofrequency Remapping Scheme

We capture degenerate frequencies by casting the frequency remapping scheme itself as **the solution to an integer linear programming problem over an integer convex cone** and exploit **the minimizing property of a Hilbert basis**. In the following discussion, we fix a truncation scheme $\mathcal{T}$. We are guided by the simple fact that $\vec{\alpha} \cdot \vec{\omega} = \vec{\beta} \cdot \vec{\omega} \iff (\vec{\alpha} - \vec{\beta}) \cdot \vec{\omega} = 0$.

Hence, two necessary and sufficient properties of a frequency remapping candidate $\vec{\eta}$ for a remapping scheme $\vec{\omega} \mapsto \vec{\eta}$ are:

$$(\vec{\alpha} - \vec{\beta}) \cdot \vec{\omega} = 0 \iff (\vec{\alpha} - \vec{\beta}) \cdot \vec{\eta} = 0 \quad \text{preserve degenerate frequencies} \qquad (4)$$

$$(\vec{\alpha} - \vec{\beta}) \cdot \vec{\omega} \neq 0 \iff (\vec{\alpha} - \vec{\beta}) \cdot \vec{\eta} \neq 0 \quad \text{do not introduce new degenerate frequencies} \qquad (5)$$

for all $\vec{\alpha}, \vec{\beta} \in \mathcal{T}$. Strengthening condition (5) by choosing an appropriate sign, we choose to enforce

$$(\vec{\alpha} - \vec{\beta}) \cdot \vec{\omega} > 0 \iff (\vec{\alpha} - \vec{\beta}) \cdot \vec{\eta} > 0. \qquad (6)$$

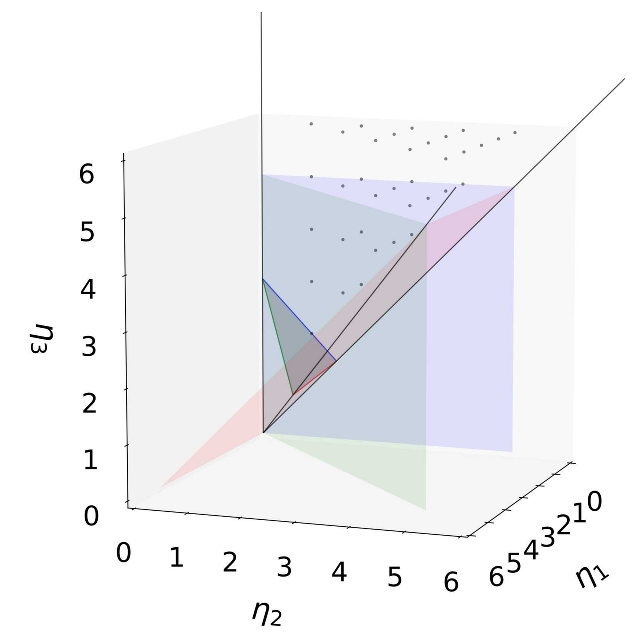
Observe that candidates $\vec{\eta}, \vec{\mu}$ satisfying (4) and (6) form a **positive convex cone** in $\mathbb{Z}^\ell$. For, affine combinations are respected:

$$\left. \begin{aligned} (\vec{\alpha} - \vec{\beta}) \cdot \vec{\eta} \geqq 0 \\ (\vec{\alpha} - \vec{\beta}) \cdot \vec{\mu} \geqq 0 \end{aligned} \right\} \implies (\vec{\alpha} - \vec{\beta}) \cdot (\lambda\vec{\eta} + (1 - \lambda)\vec{\mu}) \geqq 0 \quad \forall \lambda \in [0, 1]. \qquad (7)$$

We seek $\vec{\eta}$ such that $|\vec{\eta}|_\infty \ll |\vec{\omega}|_\infty$ to minimize the number of time collocation points for the Discrete Fourier Transform in (3).

Algorithm

1. From $\mathcal{T}$, form $\mathcal{S} = \{s_{\alpha\beta} := \vec{\alpha} - \vec{\beta} | \vec{\alpha}, \vec{\beta} \in \mathcal{T} \text{ and } (\vec{\alpha} - \vec{\beta}) \cdot \vec{\omega} > 0\}$
2. Define the annihilators $\mathcal{A} := \{s \in \mathcal{S} | s \cdot \vec{\omega} = 0\}$ and non-annihilators $\mathcal{N} := \mathcal{S} \setminus \mathcal{A}$.
3. Define the convex integer cone $\mathcal{C} \subset \mathbb{Z}^\ell$ by $n \cdot \vec{\zeta} > 0, \forall n \in \mathcal{N}$ and $a \cdot \vec{\zeta} = 0, \forall a \in \mathcal{A}$.
4. Determine a Hilbert basis $\mathcal{H}$ for $\mathcal{C}$, well-defined because $\mathcal{C} \neq \emptyset$ since $\vec{\omega} \in \mathcal{C}$. All elements of $\mathcal{C}$ are expressible as linear combinations of elements of $\mathcal{H}$.
5. Minimize the $\{-1, 0, +1\}$ combinations of elements of $\mathcal{H}$. Choose a minimizer $\vec{\eta}_0$ among these $3^{|\mathcal{H}|} - 1$ non-trivial frequencies as the remapping candidate. We call the mapping $\vec{\omega} \mapsto \vec{\eta}_0$ an **isofrequency remapping**.



Example: multi-tone application

Appying our algorithm, a 5^{th} order box truncation with

$$\vec{\omega} = (0.12 \text{ MHz}, 1.11 \text{ MHz}, 1.2 \text{ MHz})$$

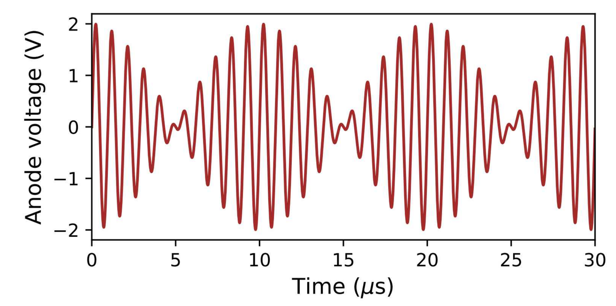
can preserve degenerate frequencies without introducing new degeneracies by using the remapping $\vec{\omega} \mapsto \vec{\eta}$ where

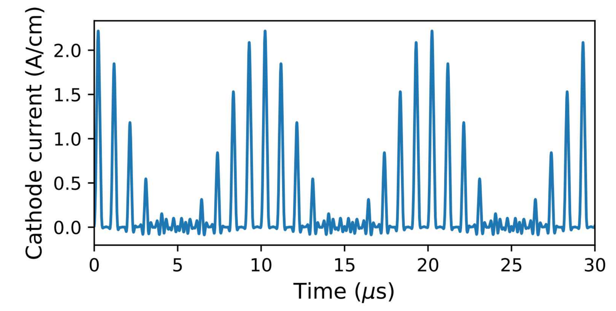
$$\vec{\eta} = (4 \text{ Hz}, 37 \text{ Hz}, 40 \text{ Hz})$$

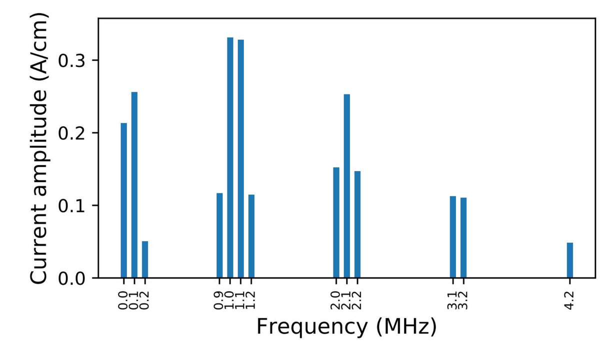
Here, $\vec{\alpha} = (2, 1, 4)$ and $\vec{\beta} = (5, 5, 0)$ correspond to 6.15 MHz.

Example: high-frequency, multi-tone problem

Applying our remapping, **Charon**'s harmonic balance method correctly captures the modulation response of a PN diode under a two-tone, high-frequency stimulus:







Summary

Traditional frequency remapping methods do not address degenerate frequencies arising in harmonic balance methods, and so can produce inaccurate problem formulations. We have designed an isofrequency remapping method in order to overcome degenerate frequencies so that the harmonic balance method may still be leveraged to accurately solve high-frequency or great frequency problems.

[1] Charon website. https://charon.sandia.gov
[2] B. Troyanovsky, Frequency Domain Algorithms for Simulating Large Signal Distortion in Semiconductor Devices, Ph.D. Thesis, Nov. 1997.
[3] J. C. Pedro and N. B. Carvalho, Efficient Harmonic Balance Computation of Microwave Circuits Response to Multi-Tone Spectra, 29th European Microwave Conference Proc., vol. I, pp.103-106, Munich, Oct.1999
[4] D. Hente and R.H. Jansen, Frequency domain continuation method for the analysis and stability investigation of nonlinear microwave circuits, IEEE Proceedings, part H, vol.133, no.5, pp.351-362, Oct.1986

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energys National Nuclear Security Administration under contract DE-NA-0003525.

U.S. DEPARTMENT OF ENERGY · NNSA National Nuclear Security Administration · CHARON