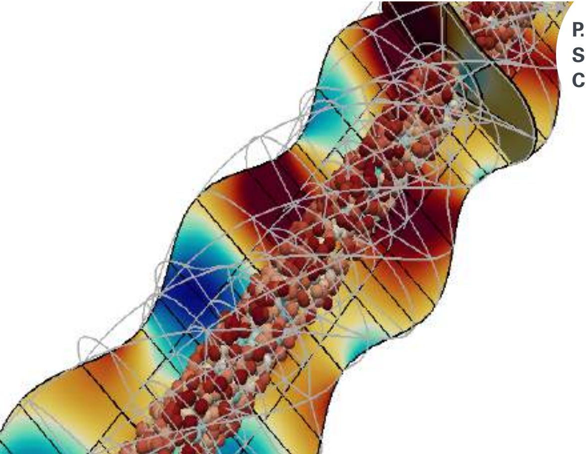

P. Ortwein
S. Copplestone
C.-D. Munz

CHALLENGING APPLICATIONS REGARDING THE SIMULATION OF MICROWAVE DEVICES

IAG, University of Stuttgart

29th Jound Russian-German Workshop

on ECHR and Gyrotrons, 2017

Development

Plasma Kinetic Code
PICLas
STUTTGART

- **Joint cooperation**[*] of Institute of Space Systems (IRS) and Institute of Aerodynamics and Gas Dynamics (IAG)
- Development and Developer
    - DSMC @ IRS: T. Binder, M. Pfeiffer, A. Mirza, P. Nizenkov, W. Reschke, S. Fasoulas
    - PIC @ IAG: S. Copplestone, P. Ortwein, C.-D. Munz

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[*] Claus-Dieter Munz et al. “Coupled particle-in-cell and direct simulation Monte Carlo method for simulating reactive plasma flows”. In: *Comptes Rendus Mécanique* 342.10 (2014), pp. 662–670.

Outline

- Brief introduction into numerics
- From simple to more complex (geometry & numeric)
  - Coaxial cable
  - Impact of PML (30 GHz gyrotron)
  - Model 140 GHz gyrotron
  - Gyro-BWO
  - Gyro-TWT
- Summary

Physical Model

1

Boltzmann Equation

Most general expression of a dilute collisional plasma

$$\left(\frac{\partial}{\partial t}+\overbrace{\vec{v}\cdot\nabla_{\vec{x}}}^{\text{convection}}+\overbrace{\frac{\vec{F_L}}{m}\cdot\nabla_{\vec{v}}}^{\text{Lorentz force}}\right)f^s(\vec{x},\vec{v},t)=\underbrace{\left.\frac{\partial f}{\partial t}\right|_{Coll}}_{\text{binary collisions}}$$

- $\vec{x}$: space coordinates
- $\vec{v}$: velocity coordinates
- t: time
- $f^s(\vec{x},\vec{v},t)$: probability density function (PDF), six-dimensional + time

The evolution of f depends on

- The velocities of particles and their spatial distribution and
- Binary collisions like relaxation processes or chemical reactions and
- The acceleration of particles due to the Lorentz forces

$$\vec{F_L}=q\left[\vec{E}(\vec{x},t)+\vec{v}\times\vec{B}(\vec{x},t)\right]$$

Numerical Model

2

Kinetic Approach

Approximation of the probability density function by a certain number of simulated particles

$$f(\vec{x},\vec{v},t) = \sum_{k=1}^{N} w_k \delta(\vec{x}-\vec{x}_k(t))\delta(\vec{v}-\vec{v}_k(t)).$$

- w_k: particle weight
- q: charge
- m_0: intrinsic mass

For each particle the relativistic equation of motion is solved

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$$

$$\frac{\mathrm{d}\gamma\vec{v}}{\mathrm{d}t} = \frac{q}{m_0}\left[\vec{E} + \vec{v} \times \vec{B}\right]$$

with Lorentz factor

$$\gamma = \frac{1}{\sqrt{1-|\vec{v}|^2/c^2}}$$

Hyperbolic-Parabolic Maxwell's Equations

By the use of Lagrange multipliers, Maxwell's Equations are modified to include the divergence constraints ($\nabla \cdot \vec{E} = \tilde{\rho}$ and $\nabla \cdot \vec{B} = 0$).[*][†]

$$\begin{aligned}
\frac{\partial \vec{E}}{\partial t} &= c^2 \, \nabla \times \vec{B} - \chi \, c^2 \, \nabla \Psi - \frac{\vec{j}}{\varepsilon_0} \\
\frac{\partial \vec{B}}{\partial t} &= - \nabla \times \vec{E} - \chi \, \nabla \Phi \\
\frac{\partial \Phi}{\partial t} &= - \chi \, c^2 \, \nabla \cdot \vec{B} - \kappa \Phi \\
\frac{\partial \Psi}{\partial t} &= - \chi \, \nabla \cdot \vec{E} + \chi \, \frac{\varrho}{\varepsilon_0} - \kappa \Psi
\end{aligned}$$

- χ: multiplier for divergence correction, generally $\chi \in [1; 10)$
- κ: parabolic damping coefficient
- Scalar correction potentials for
  - Φ: Magnetic field
  - Ψ: Electric Field

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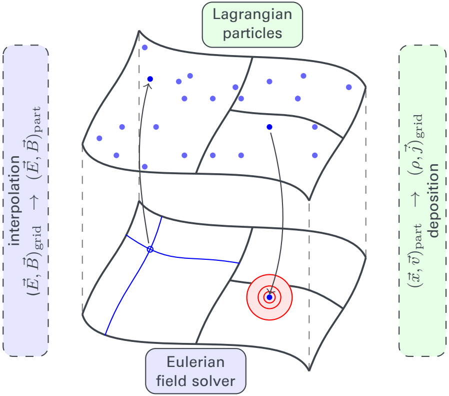
[*] C.-D. Munz et al. "Divergence Correction Techniques for Maxwell Solvers Based on a Hyperbolic Model". In: *J. of Comp. Phys.* 161.2 (2000), pp. 484–511.

[†] A. Dedner et al. "Hyperbolic Divergence Cleaning for the MHD Equations". In: *J. of Comp. Phys.* 175.2 (2002), pp. 645–673.

Particle-in-Cell



Particle Solver

- Lagrangian
- Relativistic equation of motion
- Mesh free, bounded by boundary

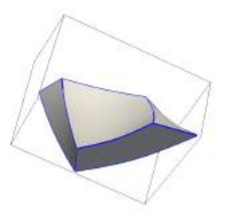
Field Solver

- Grid based
- Transformation on reference element
- Discontinuous Galerkin Spectral Element Method
- Parallelization via domain decomposition

Mesh

High-order preprocessor (HOPR)

- Mesh generator for simple geometries
- Preprocessor for mesh-tools
    - Star or CGNS format



Mesh Curving

- In-build
- Super-sampling of curved surfaces
- Agglomeration

Attributes

- Unstructured
- Non-conform
- Hexahedral mesh
- Represented by a polynomial

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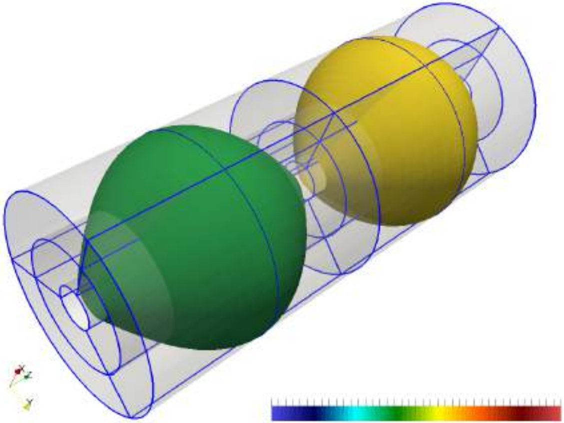
[*] F. Hindenlang, T. Bolemann, and C-D. Munz. “Mesh Curving Techniques for High Order Discontinuous Galerkin Simulations”. In: *IDIHOM: Industrialization of High-Order Methods-A Top-Down Approach*. Springer, Jan. 1, 2015, pp. 133–152.

Coaxial Cable

3

Coaxial Cable

- Simple
- TEM$_{0,0}$
- Curved Mesh:
  3 azimuthal
  2 radial
  4 z
  24 elements
  N = 11
  N$_{\mathrm{Geo}}$=11
- Exact solution
  L_2 error norm
- Investigate performance of scheme



What happens with linear elements? - OR- How to Achieve a High Accuracy?

Now:

- Linear elements $\mathcal{O}2$
- Kinks between linear elements
- Each kink excites a wave/error
- Visualize error at kinks
- L_2 error
  root mean square deviation
  (RMSD)

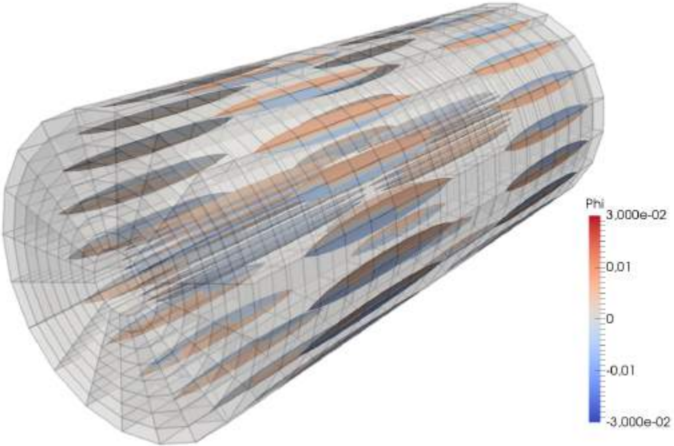


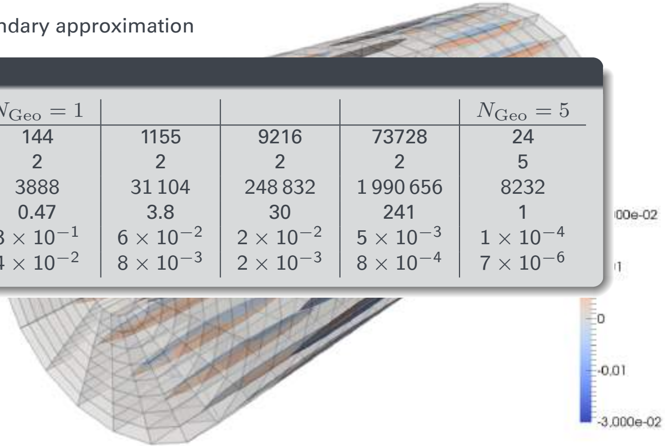
Figure: Visualization of divergence error at kinks

What happens with linear elements? - OR- How to Achieve a High Accuracy?

Dominant error: Boundary approximation

Results

	$N_{\mathrm{Geo}} = 1$				$N_{\mathrm{Geo}} = 5$
Elems	144	1155	9216	73728	24
N	2	2	2	2	5
DOF	3888	31 104	248 832	1 990 656	8232
DOF / DOF($\mathcal{O}6$)	0.47	3.8	30	241	1
$L_{2,\mathrm{E_x}} \approx$	3×10^{-1}	6×10^{-2}	2×10^{-2}	5×10^{-3}	1×10^{-4}
$L_{2,\mathrm{B_z}} \approx$	4×10^{-2}	8×10^{-3}	2×10^{-3}	8×10^{-4}	7×10^{-6}



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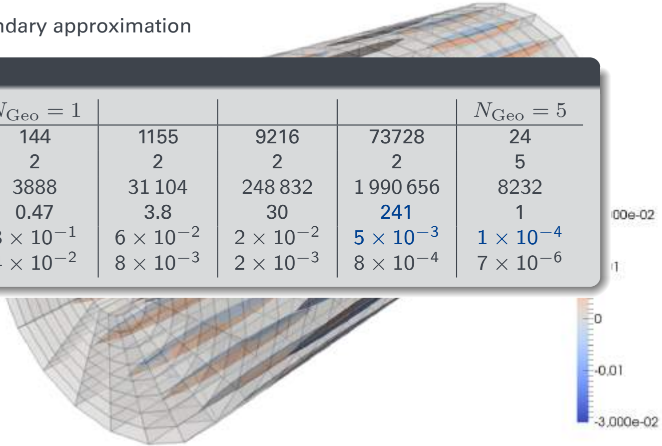


Figure: Visualization of divergence error at kinks

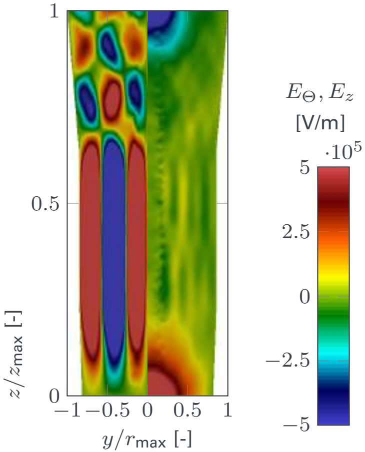
30 GHz Gyrotron

4

30 GHz Gyrotron - Impact of Perfectly Matched Layers

- Banchmark example[*,†]
  - $\text{TE}_{2,3}$ mode at $f_{RF} = 30$ GHz
- PML prevent reflections[‡]
  - Visible in output power
  - Field disturbance due to reflections
  - Static E_z due to space charge

a) no PML



Operation Parameters

- beam voltage: 79 kV
- $\alpha = \frac{v_\perp}{v_\parallel} = 1.5$
- $B_z = 1.16$ T
- $r_{beam} = 2.895$ mm

---

[*] S. Illy. “Untersuchungen von Strahlinstabilitäten in der Kompressionszone von Gyrotron-Oszillatoren mit Hilfe der kinetischen Theorie und zeitabhängiger Particle-in-Cell-Simulationen”. PhD thesis. Forschungszentrum Karlsruhe, 1997, p. 149.

[†] A. Stock et al. “Three-Dimensional Numerical Simulation of a 30GHz Gyrotron Resonator with an Explicit High-Order Discontinuous Galerkin based Parallel Particle-On-Cell Method”. In: *Plasma Science, IEEE Transactions on* 40.7 (2012), pp. 1860–1870.

[‡] S. M. Copplestone, P. Ortwein, and C.-D. Munz. “Complex-Frequency Shifted PMLs for Maxwell’s Equations With Hyperbolic Divergence Cleaning and Their Application in Particle-in-Cell Codes”. In: *IEEE Transactions on Plasma Science* 45.1 (Jan. 2017), pp. 2–14.

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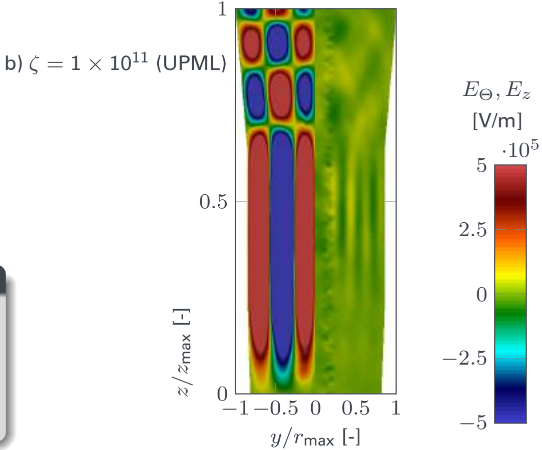

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[*] S. Illy. “Untersuchungen von Strahlinstabilitäten in der Kompressionszone von Gyrotron-Oszillatoren mit Hilfe der kinetischen Theorie und zeitabhängigner Particle-in-Cell-Simulationen”. PhD thesis. Forschungszentrum Karlsruhe, 1997, p. 149.

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140GHz Gyrotron - Down-Scaled

5

140 GHz Gyrotron

- Scale-down of a W7X-gyrotron (TE$_{28,8}$)
  - TE$_{0,3}$ mode at $f_{RF} = 140$ GHz[*]
- uniform guiding magnetic field - ACI
  - EURIDICE-q $f_0 \approx 140.30$ GHz
  - EURIDICE-q $f_1 \approx 133.95$ GHz
  - CST $f_0 \approx 140.30$ GHz
  - CST $f_0 \approx 133.70$ GHz
  - **PICLas** $f_0 \approx 140.30$ GHz
  - **PICLas** $f_1 \approx 134.04$ GHz
- non-uniform guiding magnetic field
  - EURIDICE-q $P \approx 10.3$ kW
  - EURIDICE-q $f_0 \approx 140.30$ GHz
  - CST $P \approx 9.6$ kW
  - CST $f_0 \approx 140.20$ GHz
  - **PICLas** $P \approx 9.5$ kW
  - **PICLas** $f_0 \approx 140.30$ GHz

Operation Parameters

- beam voltage: 66.64 kV
- beam current: 1 A
- $\alpha = \frac{v_\perp}{v_\parallel} = 1.3$
- $B_z = 5.561$ T
- $r_{beam} = 0.624$ mm
- $r_{cut,cavity} = 140.02$ GHz

Costs $\mathcal{O}6$

- 50 CPUh per 1 ns
- 60 cores
- No efficiency study

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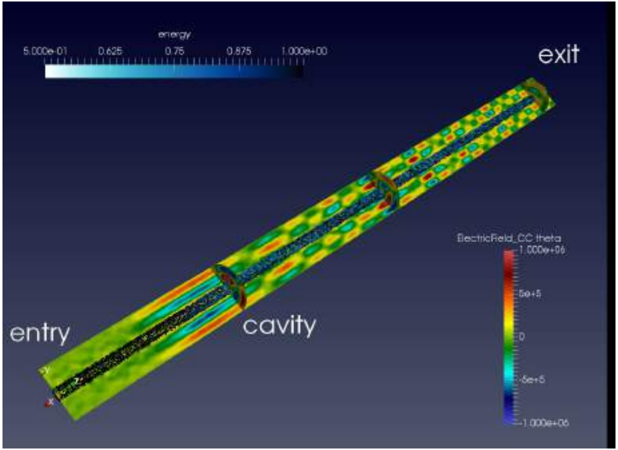
[*] K. A. Avramidis et al. “A comparative study on the modeling of dynamic after-cavity interaction in gyrotrons”. In: *Phys. Plasmas* 22.5 (May 2015).

140 GHz Gyrotron

Movie

- Empty domain
- First excitation
  cavity & uptaper
- $\mathrm{TE}2,3 \rightarrow \mathrm{TE}1,3 \rightarrow \mathrm{TE}0,3$
- Particles energy
  Smaller energy -> larger size



Gyrotron Backward-Wave Oscillator

6

Setup

- Corrugations

$$r(\phi, z) = r_0 + \tilde{r} \cos\left(m\phi - \frac{2\pi}{z}\right),$$

parameter	value
r_0 / mm	0.534
$\tilde{r}$ / mm	0.085
d / mm	1.06
m_b / -	-3

- 18 regular periods
- 3 period taper (input & output)
- 1 period waveguide (PML)

- Beam parameter

parameter	value
current / A	0.7
voltage / kV	30
pitch factor / -	1.3
$B_{\text{z,guiding}}$ / T	4.991

- Numerical parameter

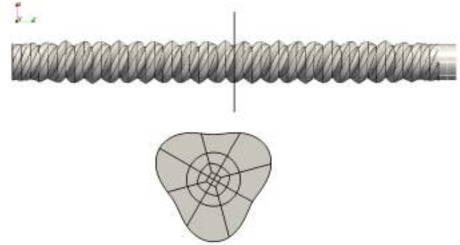
parameter	value
N / -	5
particle weight / -	1×10^4
ζ / -	260×10^9
α_0 / -	0

Mesh

- Deformed waveguide
- Helical corrugations

$$r(\phi, z) = r_0 + \tilde{r}\cos\left(m\phi - \frac{2\pi}{z}\right)$$

- Computational grid $\mathcal{O}5$, 2400 elements



Motivation

- Complex geometry
- Curvilinear & 3D
  → Test for numerics

Meshing

- Meshed by High-Order Preprocessor (HOPR), open-source
- In-build function
- Order of mesh representation can be chosen freely
- Challenge for high-order methods: $d \approx \lambda$

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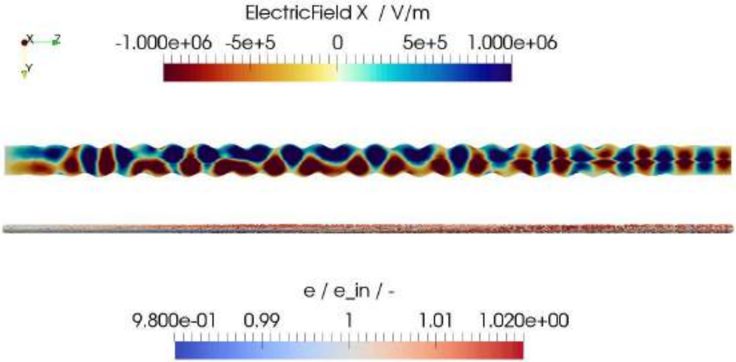
[*] F. Hindenlang, T. Bolemann, and C-D. Munz. "Mesh Curving Techniques for High Order Discontinuous Galerkin Simulations". In: *IDIHOM: Industrialization of High-Order Methods-A Top-Down Approach*. Springer, Jan. 1, 2015, pp. 133–152.

It’s Time For a Movie

Details

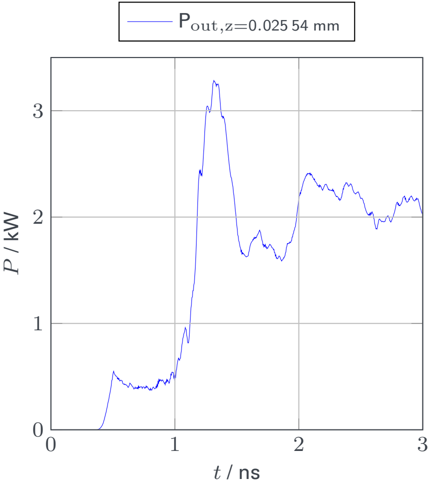
- Start-Time:
  3 ns
- 24 samples per RF-period
- $f \approx 260$ GHz
- Steady-state



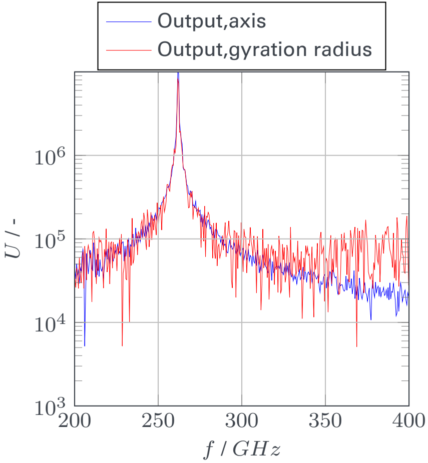
Power Output

Infos

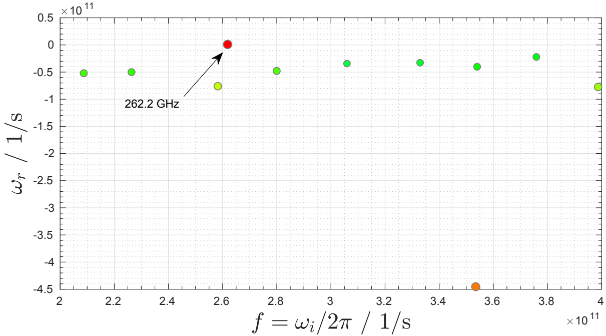
- Flux of Poynting vector in axial direction
- Averaged over one f_{RF} period
- CFS-PML
  $\zeta = 260 \times 10^9$, $\alpha = 0$
- Output power
  $P_{\mathrm{out}} \approx 2.1$ kW



FFT vs. DMD



- Peak at $f = 261.7$ GHz



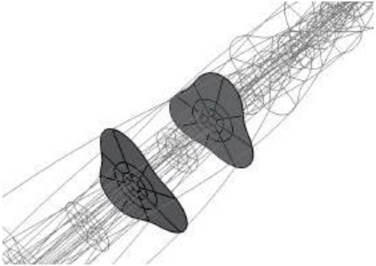
- Peak at $f = 262.2$ GHz
- Whole domain

Gyro-TWT

7

Cold Simulation

Investigated design: $TE_{1,1}$[*],[†]



- Fully curvilinear
- Twisted mesh to follow corrugations
- (Non-conforming mesh: local refinement)
- Here: Refinement at particle orbit

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[*] N. S. Ginzburg et al. “Chaotic millimeter wave generation in a helical-waveguide gyro-TWT with delayed feedback”. In: *Physics of Plasmas* 23.10 (2016), pp. 1089–7674.

[†] S. V. Samsonov et al. “Ka-Band Gyrotron Traveling-Wave Tubes With the Highest Continuous-Wave and Average Power”. In: *IEEE Transactions on Electron Devices* 61.12 (Dec. 2014), pp. 4264–4267.

Setup

- Corrugations

$$r(\phi, z) = r_0 + \tilde{r}\cos\left(m\phi - \frac{2\pi}{z}\right)$$

parameter	value
r_0 / mm	4
$\tilde{r}$ / mm	0.74
d / mm	9.2
m_b / -	3

- 15 regular periods
- 2 period taper (input & output)
- 1 period circular waveguide (input)
- 1 period circular waveguide (exit)
- 1 period circular waveguide (PML)

- Beam parameter

parameter	value
current / A	10
voltage / kV	70
pitch factor / -	1.2
$B_{\text{z,guiding}}$ / T	0.65

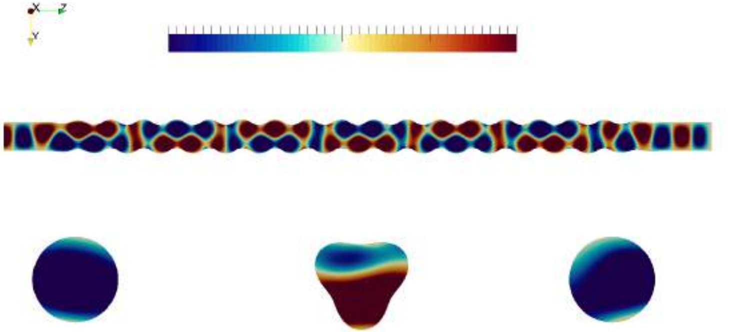
- Numerical parameter

parameter	value
N / -	5
particle weight / -	1×10^4
ζ / -	350×10^9
α_0 / -	35×10^9

Cold Simulation

Details

- Start-Time: 40 ns
- 24 samples per RF-period
- $f = 35$ GHz
- Steady-state
- Left input
- Right PML



Summary

8

Summary

- **PICLas**
  - Discontinuous Galerkin spectral element method
  - High-order conforming (or non-conforming) curvilinear hex-meshes
- **Increasing complexity**
  - Coaxial cable to emphasis impact of high-order
  - 30 GHz gyrotron TE$_{2,3}$
  - model 140 GHz gyrotron TE$_{0,3}$
  - Gyro-BWO
  - Cold simulations of gyro-TWT
- **Outlook**
  - Hot simulations of gyrotron Traveling Wave Tube
  - Non-conforming meshes

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IAG, German-Russian Workshop, Stuttgart, 2017

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Current Problems With and Without Particles

- Geometry issue?
  - Using a pulsed TE$_{1,1}$ wave
    Backwards propagating wave at the first transition from left to right rotating mode
    Physical correct or error?
- How to insert mode and particles?
  Change of reflections/excitation of wrong modes
- Currently: constant guiding magnetic field
- How to start-up simulation?
  a) First particles, than TE wave
  b) First TE wave, than particles