Dynamical Systems Bifurcation Analysis of FDTD Methods in Nonlinear Optical Materials

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Abstract

Previous approaches [1] to solving Maxwell's equations in non-linear media including Lorentz, Kerr and Raman interactions have required a compute intensive non-linear equation solution step. Similar to the approach presented in [4] in this paper we present a FDTD scheme which formulates the displacement current equations in a manner which avoids this overhead. Energy estimates confirm the stability of our proposed method. Moreover, a dynamical system bifurcation analysis of the scheme for a travelling plane wave demonstrates that the proposed scheme is able to capture the bifurcation of the continuous PDE. Numerical experiments are also presented.

Maxwell's Equations for Nonlinear Kerr and Raman Effects

Maxwell's equations in a non-magnetic, non-conductive, non-linear dispersive medium $\mathcal{D} \subset \mathbb{R}^3$ governing the electric field $\mathbf{E}$ and the magnetic field $\mathbf{H}$ for time $t \in [0, T]$ for $T > 0$:

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = \mathbf{0}, \text{ in } (0,T] \times \mathcal{D},$$

$$\partial_t \mathbf{D} - \nabla \times \mathbf{H} = \mathbf{0}, \text{ in } (0,T] \times \mathcal{D},$$

$$\nabla \cdot \mathbf{B} = 0,\ \nabla \cdot \mathbf{D} = 0, \text{ in } (0,T] \times \mathcal{D},$$

Constitutive Laws:

$$\mathbf{D} = \epsilon_0 (\overbrace{\epsilon_\infty \mathbf{E}}^{\text{Linear, Instantaneous}} + \overbrace{\mathbf{P}}^{\text{Linear Dispersion}} + \overbrace{a(1-\theta)\mathbf{E}||\mathbf{E}||_2^2}^{\text{Nonlinear Instantaneous Kerr}} + \overbrace{a\theta Q\mathbf{E}}^{\text{Nonlinear dispersion}}),$$
$$\mathbf{B} = \mu_0 \mathbf{H}.$$

Sellmeir Relations: For anisotropic crystals, where the principal optical axis is aligned with the laboratory co-ordinates, Bourgeade and Nkonga, present a simplified model in [2]. The dispersive linear polarization $\mathbf{P}^{(1)}_{\text{disp}}$ is characterized by two Lorentz resonances (indexed by a and b):

$$\begin{aligned}
\mu_0 \tfrac{\partial H}{\partial t} &= \tfrac{\partial E}{\partial z} \\
\tfrac{\partial D}{\partial t} &= \tfrac{\partial H}{\partial z} \\
D &= \epsilon_0(\epsilon_\infty E + \alpha_a F + \alpha_b G) + P \\
\tfrac{\partial F}{\partial t} &= J_F \\
\tfrac{\partial J_F}{\partial t} + \delta_a J_F + \omega_a^2 F &= \omega_a^2 \chi_a E \\
\tfrac{\partial G}{\partial t} &= J_G \\
\tfrac{\partial J_G}{\partial t} + \delta_b J_G + \omega_b^2 G &= \omega_b^2 \chi_b E \\
\tfrac{\partial P}{\partial t} &= J_P \\
\tfrac{\partial J_P}{\partial t} + \delta J_P + \omega_0^2 P &= \epsilon_0 \left(\beta E^2 + \gamma E^3\right)
\end{aligned}$$

where ω_a and ω_b are angular verilocity tensors associated with the Lorentz frequencies, δ_a and δ_b are the corresponding damping tensors, and χ_d is a material specific tensor, which highlights the optical property of the material.

Energy Identity for Continuous Model

Given a nonlinear anisotropic medium Ω, with periodic boundary conditions for all fields, the nonlinear Maxwell's equations given above satisfy the following energy identity.

Theorem (Energy Identity)

Given Ω, with periodic boundary conditions:

$$\frac{d}{dt}E(t) = -\int_{\partial\Omega} (E \times H) \cdot \mathbf{n}\, d\sigma - \epsilon_0 \int_\Omega \left(\left(\frac{\sqrt{\alpha_a \delta_a} \mathbf{J_F}}{\omega_a \sqrt{\chi_d}}\right)^2 + \left(\frac{\sqrt{\alpha_b \delta_b} \mathbf{J_G}}{\omega_b \sqrt{\chi_d}}\right)^2 + \frac{\delta \mathbf{J_P}^2}{\omega_0^2(\beta E + \gamma E^2)} \right) d\sigma$$

where $E(t)$ is given by:

$$E(t) = \frac{1}{2}\int_\Omega \left(\mu_0 \mathbf{H}^2 + \epsilon_0 \epsilon_\infty \mathbf{E}^2 + \frac{\epsilon_0 \alpha_a \mathbf{J_F}^2}{\chi_d \omega_a^2} + \frac{\epsilon_0 \alpha_a \mathbf{F}^2}{\chi_d} + \frac{\epsilon_0 \alpha_b \mathbf{J_G}^2}{\chi_d \omega_b^2} + \frac{\epsilon_0 \alpha_b \mathbf{G}^2}{\chi_d} + \frac{\epsilon_0 \mathbf{J_P}^2}{\omega_0^2(\beta E + \gamma E^2)} + \frac{\epsilon_0 \mathbf{P}^2}{\beta E + \gamma E^2} \right) d\sigma$$

Energy Decay for the Discrete Nonlinear Maxwell Model

The average power transmitted in Maxwell's wave equation can be modelled using the Poynting vector as

$$S_{\text{av}} = \frac{1}{2}\text{Re}(E \times H^*)$$

Given $\nabla \times E = i\omega\mu H$ from the time harmonic wave equation, we multiply by H^*, the complex conjugate of H. Similarly, given $\nabla \times H^* = i\omega\epsilon_c^* E^* + J^*$, we multiply by E and subtract to get:

$$H^* \cdot (\nabla \times E) - E \cdot (\nabla \times H^*) \ = \ \nabla \cdot (E \times H^*) = (\sigma + \omega\epsilon)||E||^2 + EJ^* - i\omega\mu||H||^2$$

We would like to get an equivalent identity for the discrete finite difference equations. Let $H_h^{n+1/2} \in V_{1/2,h}$ while $E_h^n, P_j^n \in V_{0,h}$, and particular to our proposed method is $J_{j+1/2}^{n+1/2} \in V_{1/2,1/2h}$. Define $\mathcal{A} = \tilde{D}_{1,h}^{(2M)} \circ D_{1,h}^{(2M)}$, which is a $(2M)$ order finite difference approximation of the 1D Laplacian operator. It is shown in [3] that $\mathcal{A}$ operator is positive,

Theorem (Energy Decay)

$$\begin{aligned}
&\mathcal{E}^{n+1/2}(t) + \epsilon_0\left(\frac{\delta_a \mathbf{J_F}^2}{\omega_a^2} + \frac{\delta_b \mathbf{J_G}^2}{\omega_b^2} + \frac{\delta \mathbf{J_P}^2}{\omega_0^2(\beta E + \gamma E^2)}\right) = -\sum_{j=0}^{I-1} \Big[\mu_0 ||H_j^{n+1/2}||^2 \\
&+ \ \epsilon_0 (< E_j^{n+1/2}, (I_h + \frac{c^2 \Delta t^2}{4} \mathcal{A}_{1,h}^{(2M)}) E_j^{n+1/2} >_{0,h} + \frac{\alpha_a (J_{F_j}^{n+1/2})^2}{\chi_d \omega_a^2} + \frac{\alpha_a (F_j^{n+1/2})^2}{\chi_d} \\
&+ \ \frac{\alpha_b (J_{G_j}^{n+1/2})^2}{\chi_d \omega_b^2} + \frac{\alpha_b (G_j^{n+1/2})^2}{\chi_d} + \frac{(J_{P_j}^{n+1/2})^2}{\omega_0^2(\beta E + \gamma E^2)} + \frac{(P_j^{n+1/2})^2}{\beta E_j^n + \gamma (E_j^n)^2} \Big]
\end{aligned}$$

As can be seen in the above equation, the scheme is stable, and moreover when $\delta_a \to 0$ and $\delta_b \to 0$, and $\beta = 0$ (this is the case for centro-symmetric media) the discrete scheme is conservative.

2M Order Spatial Approximations

Finite dimensional discrete space

◇ Space of discrete electric fields

$$V_{0,h}^{\Omega} := \left\{ E = (E_i) |\ \ x_i \in G_{p,\Omega},\ E_0 = E_I, ||E||^2_{0,h,\Omega} = h \sum_{l=0}^{I-1} |E_\ell|^2 < \infty \right\},$$

◇ Space of discrete magnetic fields

$$V_{\frac{1}{2},h}^{\Omega} := \left\{ H = (H_{i+\frac{1}{2}}) |\ x_{i+\frac{1}{2}} \in G_{d,\Omega}, ||H||^2_{\frac{1}{2},h,\Omega} = h \sum_{\ell=0}^{I-1} |H_{\ell+\frac{1}{2}}|^2 < \infty \right\}.$$

Finite difference approximation

$$\begin{aligned}
\frac{\mathbf{P}_j^{n+1} - \mathbf{P}_j^n}{\Delta t} &= \mathbf{J}_j^{n+1/2} \\
\frac{\mathbf{J}_j^{n+1/2} - \mathbf{J}_j^{n-1/2}}{\Delta t} &= \omega_0^2 \epsilon_0 (\beta (E_j^n)^2 + \gamma (E_j^n)^3) - \omega_0^2 \mathbf{P}_j^n \\
\frac{\mathbf{H}_{j+1/2}^{n+1/2} - \mathbf{H}_{j+1/2}^{n-1/2}}{\Delta t} &= \frac{1}{\mu_0}\Big[(D_{1,h}^{(2M)} E)_j^n\Big] \\
\frac{\mathbf{E}_j^{n+1} - \mathbf{E}_j^n}{\Delta t} &= \frac{1}{\epsilon_0}\Big[(\tilde{D}_{1,h}^{(2M)} H)_j^{n+1/2} - J_j^{n+1/2} - J_{F_j}^{n+1/2} - J_{G_j}^{n+1/2}\Big] \\
\frac{\mathbf{F}_k^{n+1} - \mathbf{F}_k^n}{\Delta t} &= \mathbf{J}_{F,k}^{n+1/2} \\
\frac{\mathbf{G}_k^{n+1} - \mathbf{G}_k^n}{\Delta t} &= \mathbf{J}_{G,k}^{n+1/2} \\
\frac{\mathbf{J}_{F,k}^{n+1/2} - \mathbf{J}_{F,k}^{n-1/2}}{\Delta t} &= \omega_a^2 \cdot \chi_d \cdot \mathbf{E}_k^n - \omega_a^2 \mathbf{F}_k^n \\
\frac{\mathbf{J}_{G,k}^{n+1/2} - \mathbf{J}_{G,k}^{n-1/2}}{\Delta t} &= \omega_b^2 \cdot \chi_d \cdot \mathbf{E}_k^n - \omega_b^2 \mathbf{G}_k^n
\end{aligned}$$

As can be observed the proposed FDTD scheme is full explicit, marches forward in time, and at any time internal n, does not need to solve a non-linear system of equations.

Analysis of Travelling Wave

Stable Points

Next we consider the propagation of a linearly polarized 1D plane wave, $\mathbf{E} = E(z,t)$ propagating in the z-direction. Then the form of the wave is:

$$\mathbf{E}(\mathbf{r}, t) = E_x(\mathbf{r}, t)\hat{i} = \{E_0(z,t)\exp[i(kz - \omega t)] + \text{c.c.}\}\hat{i}$$

The other fields such as $\mathbf{H}, \mathbf{P}, \mathbf{D}$, therefore also have the same form. Using the travelling wave assumption, we can write the above fields in $\xi = z - vt$ coordinate.

Theorem (Travelling Wave Propagation)

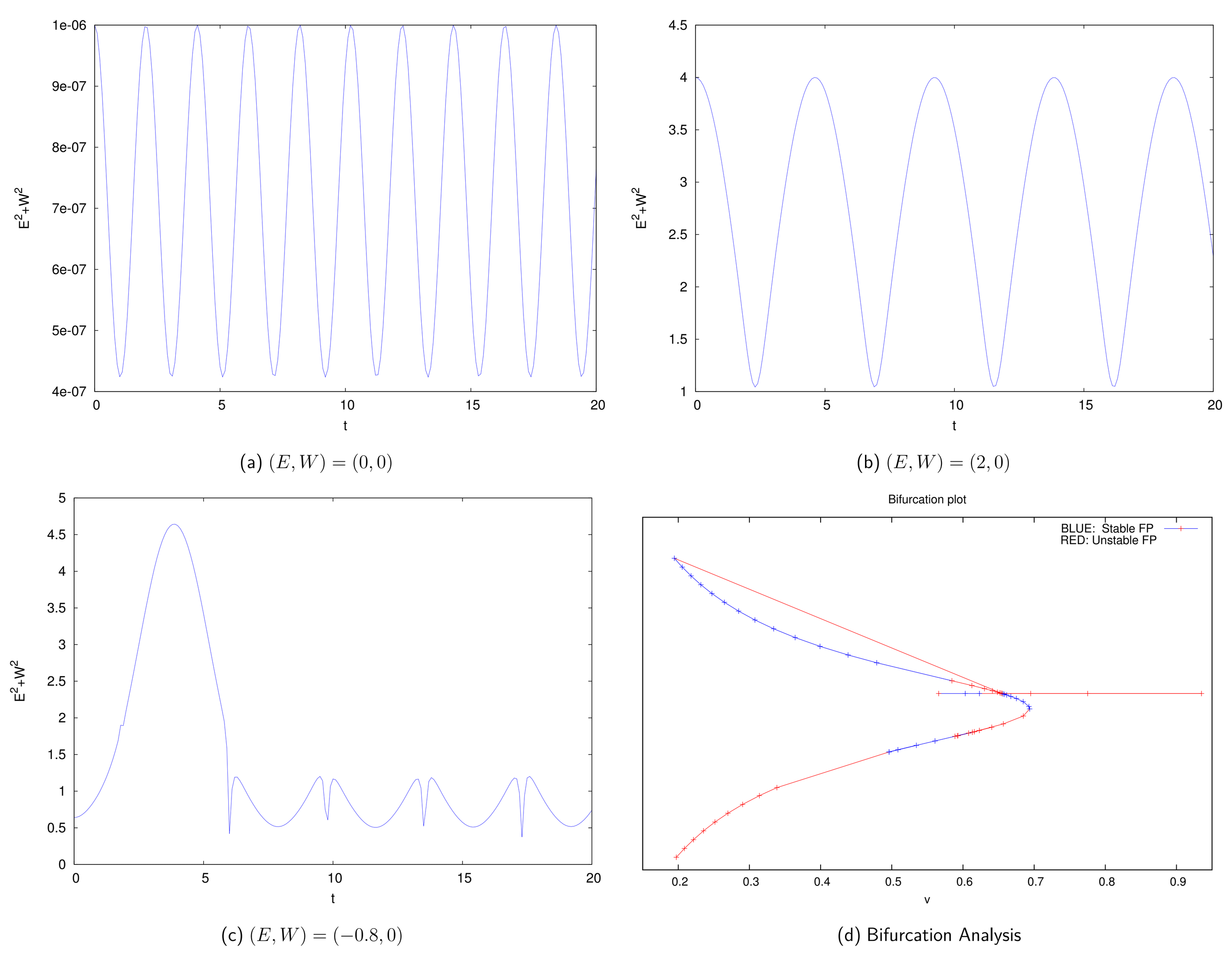
Given $\mathbf{E}$ as above, the coupled system of polarization $\mathbf{P}$ and $\mathbf{E}$ has stationary point at $(E, W) = (0,0)$, where $W = \frac{\partial E}{\partial \xi}$. The system has additional stationary points at:

$$(E, W) \ = \ \left(\frac{\omega_0^2 \left(\frac{-\beta}{\sqrt{\gamma}} \sqrt{\frac{c^2}{v^2} - \epsilon_s} + 2\frac{c^2}{v^2} - 2\epsilon_s\right)}{v^2 \left(\frac{\beta}{\sqrt{\gamma}} \sqrt{\frac{c^2}{v^2} - \epsilon_s} + 3\epsilon_s - \epsilon_\infty\right) - 2c^2}, 0\right) \qquad (0.1)$$

and

$$(E, W) \ = \ \left(\frac{\omega_0^2 \left(\frac{\beta}{\sqrt{\gamma}} \sqrt{\frac{c^2}{v^2} - \epsilon_s} + 2\frac{c^2}{v^2} - 2\epsilon_s\right)}{v^2 \left(\frac{-\beta}{\sqrt{\gamma}} \sqrt{\frac{c^2}{v^2} - \epsilon_s} + 3\epsilon_s - \epsilon_\infty\right) - 2c^2}, 0\right) \qquad (0.2)$$

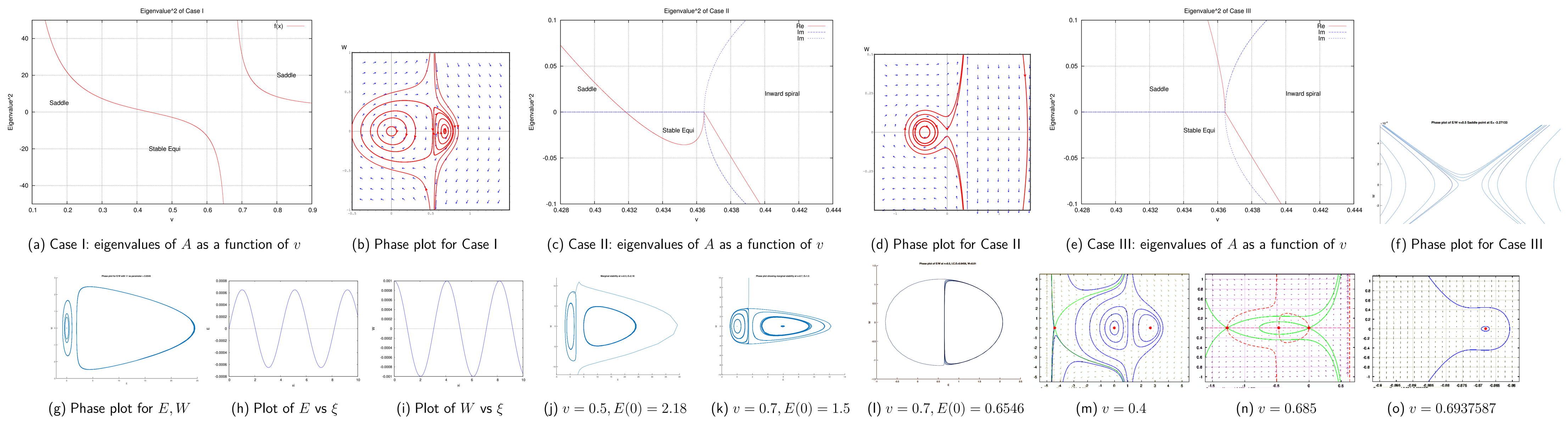
$$\frac{\partial E}{\partial \xi} = W, \ \frac{\partial W}{\partial \xi} = \frac{6\gamma E v^2 W^2 + 2\beta v^2 W^2 - E\omega_0^2[\frac{c^2}{v^2} - \epsilon_s - \beta E - \gamma E^2]}{c^2 - v^2(\epsilon_\infty + 2\beta E + 3\gamma E^2)}$$



(a) $(E, W) = (0,0)$ (b) $(E, W) = (2,0)$ (c) $(E, W) = (-0.8, 0)$ (d) Bifurcation Analysis

Figure: Lyapunov function and bifurcation analysis $r(\xi) = E^2 + W^2$ plot for case I.

Stability Regions for the Continuous Formulation



(a) Case I: eigenvalues of A as a function of v (b) Phase plot for Case I (c) Case II: eigenvalues of A as a function of v (d) Phase plot for Case II (e) Case III: eigenvalues of A as a function of v (f) Phase plot for Case III

(g) Phase plot for E, W (h) Plot of E vs ξ (i) Plot of W vs ξ (j) $v = 0.5, E(0) = 2.18$ (k) $v = 0.7, E(0) = 1.5$ (l) $v = 0.7, E(0) = 0.6546$ (m) $v = 0.4$ (n) $v = 0.685$ (o) $v = 0.6937587$

Figure: Eigenvalues of A as a function of v and phase plot of E, W around $(0,0)$

Stability Regions for the Discrete Formulation

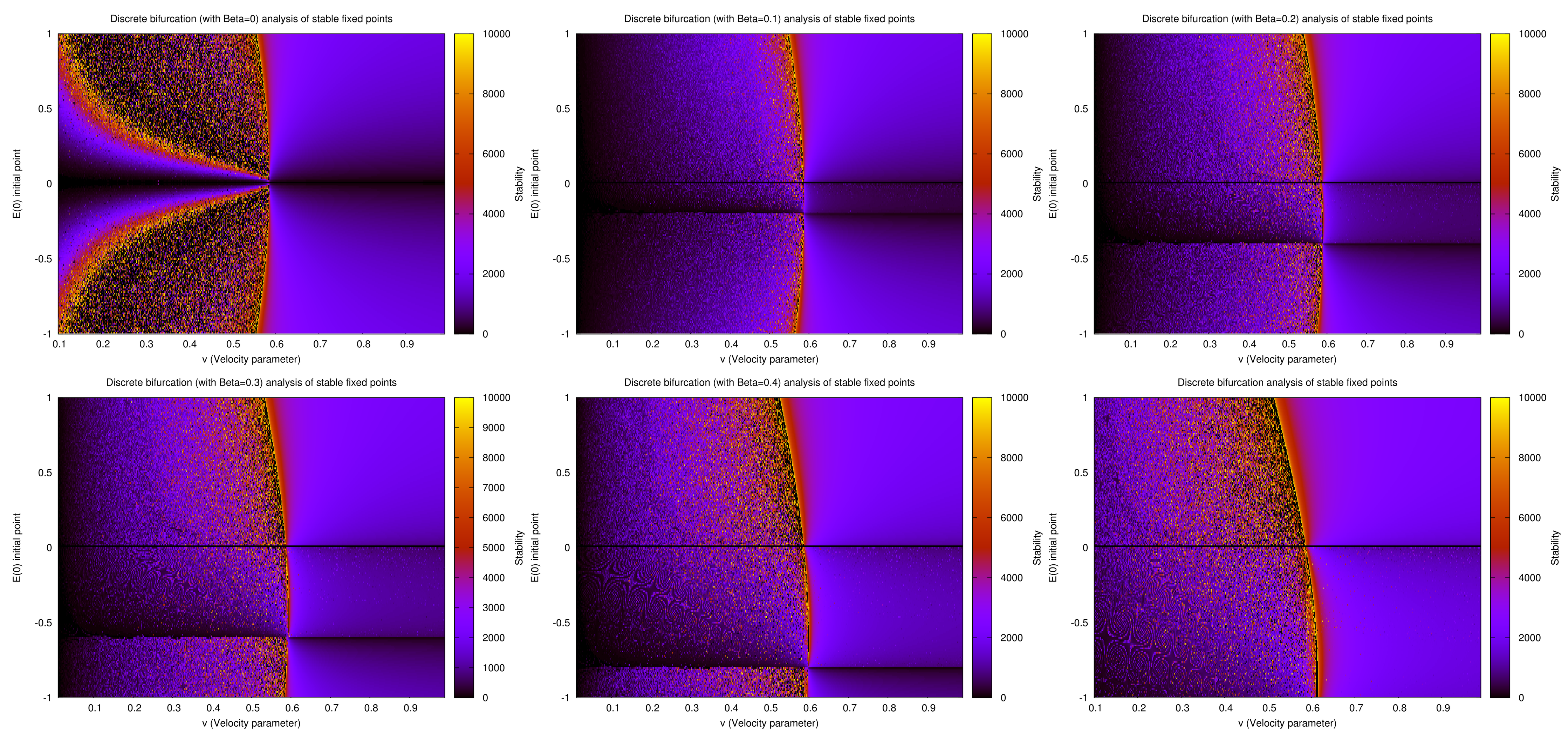


Figure: Bifurcation plot showing branch points, stable and unstable fixed points.

Fully Discrete Analysis

Consider the original form of the PDE

$$\frac{1}{v^2}E(z,t)_{tt} = E(z,t)_{zz} - g(E(z,t)) \qquad (0.3)$$

We can discretize the above using second order in space (with step h) and time (with step Δt) to get:

$$\left(\frac{1}{v^2} + 2\beta E(z,t) + 3\gamma(E(z,t))^2\right)\frac{E(z,t+\Delta t) - 2E(z,t) + E(z,t-\Delta t)}{\Delta t^2} = E(z,t)_{zz} - \Big[(2\beta + 6\gamma E(z,t))\Big(\frac{E(z,t) - E(z,t-\Delta t)}{\Delta t}\Big)^2 - E(z,t)\omega_0^2\big[\frac{c^2}{v^2} - \epsilon_s - \beta E(z,t) - \gamma(E(z,t))^2\big]\Big]$$

Now we use the travelling coordinate condition and write $\kappa = v\Delta t$.

$$\varphi(\xi + \kappa) = 2\varphi(\xi) - \varphi(\xi - \kappa) + \frac{(\varphi(\xi) - \varphi(\xi - \kappa))^2}{\frac{2\beta\varphi(\xi) + 3\gamma(\varphi(\xi))^2}{2\beta + 6\gamma\varphi(\xi)}} - \frac{(\Delta t)^2 \omega_0^2 \Big[\frac{c^2}{v^2} - \epsilon_s - \beta\varphi(\xi) - \gamma(\varphi(\xi))^2\Big]}{2\beta + 3\gamma\varphi(\xi)}$$

Numerical simulations of this discretized equation are shown in the Figure above which confirms the ability of the proposed scheme to capture the eigenvalues of the continuous scheme.

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