EFFECTIVE NUMERICAL-ANALYTICAL METHOD FOR MODELING THE DYNAMICS OF A FUEL CELL SYSTEM FOR A PULSED TYPE REACTOR

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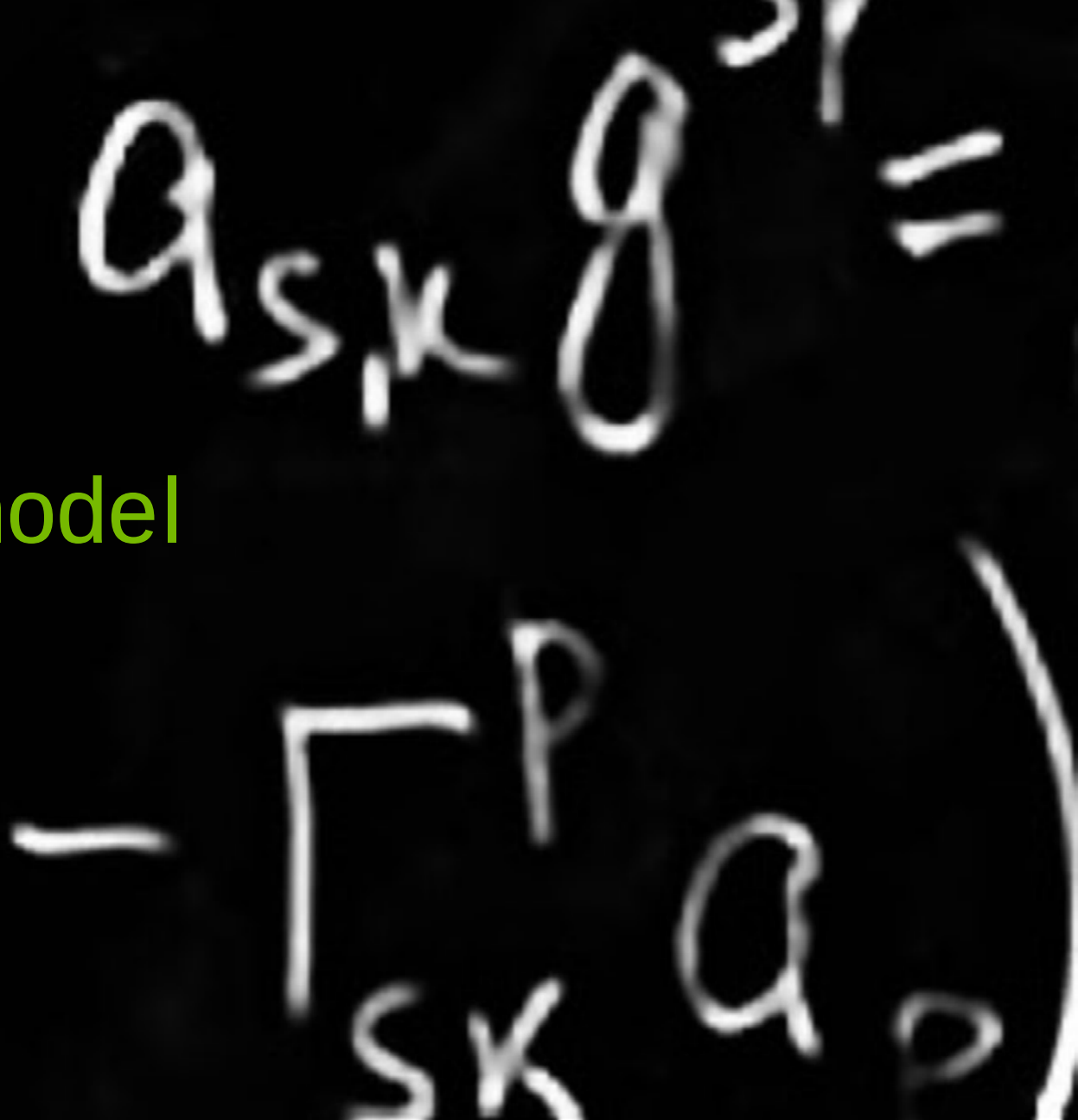
NEPTUN project

LNP JINR

OUTLINE

- Mathematical model of the FE system for the NEPTUN project
- Parallel realization by GPU
- Results

Mathematical model



ACTIVE ZONE

Generalized coordinates $\vec{r}_n = \vec{r}_n\left(q_1,...,q_{2N}\right),\ n=1...N,$

$$\left(q_1,...,q_{2N}\right)=\left(x_1,...,x_N,y_{N+1},...,y_{2N}\right)\mapsto\left(r_1,...,r_N,\varphi_{N+1},...,\varphi_{2N}\right),$$
$$\left(\dot{q}_1,...,\dot{q}_{2N}\right)=\left(\dot{x}_1,...,\dot{x}_N,\dot{y}_{N+1},...,\dot{y}_{2N}\right)\mapsto\left(\dot{r}_1,...,\dot{r}_N,\dot{\varphi}_{N+1},...,\dot{\varphi}_{2N}\right).$$

Hamiltonian function

$$H(q,p)=\sum_{n=1}^{N}\frac{1}{2m_n}\left(\left[p_n^{(r)}\right]^2+\frac{1}{r_n^2}\left[p_n^{(\varphi)}\right]^2\right)+$$
$$+\sum_{n=1}^{N}\sum_{k\in\Omega_n}\Phi\left(\sqrt{r_n^2+r_k^2-2r_nr_k\cos\left(\varphi_n-\varphi_k\right)}\right),$$

where $p_n^{(r)}=m_n\sum_{j=1}^{N}g_{n,j}\dot{q}_j,\ p_n^{(\varphi)}=m_n\sum_{j=N+1}^{2N}g_{n+N,j}\dot{q}_j,\ p_n^{(r)}=m_n\dot{r}_n,\ p_n^{(\varphi)}=m_nr_n^2\dot{\varphi}_n,$

$g_{sk}\mapsto\begin{pmatrix}\mathrm{I}_N & 0\\ 0 & G_N\end{pmatrix},\ G_N=\mathrm{diag}\left(r_1^2,...,r_N^2\right),\ \mathrm{I}_N$ *is an identity matrix.*

HAMILTONIAN FORMALISM

Canonical variables $\vec{z} = \{q_1, ..., q_{2N}, p_1, ..., p_{2N}\}^T$,

$\dot{\vec{z}} = J\partial_z H,$ where $J = \begin{pmatrix} 0 & \mathrm{I}_{2N} \\ -\mathrm{I}_{2N} & 0 \end{pmatrix}$, $\partial_z = \{\partial_{z_1}, ..., \partial_{z_{4N}}\}^T = \{\partial_{q_1}, ..., \partial_{q_{2N}}, \partial_{p_1}, ..., \partial_{p_{2N}}\}^T$.

$\vec{\eta} = \{u_1^{(r)}, ..., u_N^{(r)}, u_1^{(\varphi)}, ..., u_N^{(\varphi)}, p_1^{(r)}, ..., p_N^{(r)}, \tilde{p}_1^{(\varphi)}, ..., \tilde{p}_N^{(\varphi)}\}^T$, $u_j^{(r)} = r_j - R_j$, $u_s^{(\varphi)} = \varphi_s - \Theta_s$, $\tilde{p}_n^{(\varphi)} = p_n^{(\varphi)} / R_n$.

An approximation of Hamiltonian function

$$H_a(u,p) = \sum_{n=1}^{N} \frac{1}{2m_n} \eta_{2N+n}^2 + \sum_{n=1}^{N} \frac{1}{2m_n} \eta_{3N+n}^2 + \frac{1}{2} \sum_{j,s=1}^{N} \kappa_{j,s}^{(1,1)} \eta_j \eta_s + \frac{1}{2} \sum_{j,s=1}^{N} \kappa_{j,s}^{(1,2)} \eta_j \eta_{N+s} + \frac{1}{2} \sum_{j,s=1}^{N} \kappa_{j,s}^{(2,2)} \eta_{N+j} \eta_{N+s},$$

where $\kappa_{j,s}^{(1,1)} = \dfrac{\partial^2 U(R,\Theta)}{\partial r_j \partial r_s}$, $\kappa_{j,s}^{(1,2)} = \dfrac{\partial^2 U(R,\Theta)}{\partial r_j \partial \varphi_s}$, $\kappa_{j,s}^{(2,1)} = \kappa_{s,j}^{(1,2)}$, $\kappa_{j,s}^{(2,2)} = \dfrac{\partial^2 U(R,\Theta)}{\partial \varphi_j \partial \varphi_s}$.

Motion equations $\dot{\vec{\eta}} = J\partial_\eta H_a = \mathrm{G}\vec{\eta},$ $\partial_\eta = \{\partial_{\eta_1}, ..., \partial_{\eta_{4N}}\}^T$,

$\mathrm{G} = \begin{pmatrix} 0 & \mathrm{D} \\ -\mathrm{K} & 0 \end{pmatrix}$, $\mathrm{K} = \begin{pmatrix} \kappa^{(1,1)} & \kappa^{(1,2)} \\ \kappa^{(2,1)} & \kappa^{(2,2)} \end{pmatrix}$, $\mathrm{D} = \begin{pmatrix} d^{(1,1)} & 0 \\ 0 & d^{(2,2)} \end{pmatrix}$, $d^{(1,1)} = d^{(2,2)} = \mathrm{diag}\left(\frac{1}{m_1}, ..., \frac{1}{m_N}\right)$.

DISSIPATIVE SYSTEM

Dissipative system $L(\vec{r},\vec{v},t)=\left[\frac{mv^2}{2}-U(\vec{r})\right]e^{2\gamma t}\Rightarrow H(\vec{r},\vec{\mathrm{p}},t)=\frac{\mathrm{p}^2}{2m}e^{-2\gamma t}+U(\vec{r})e^{2\gamma t}$, *where* $\vec{\mathrm{p}}\overset{\text{def}}{=}\vec{p}e^{2\gamma t}$.

$$\vec{\eta}\overset{\text{def}}{=}\left\{u_1^{(r)},...,u_N^{(r)},u_1^{(\varphi)},...,u_N^{(\varphi)},\mathrm{p}_1^{(r)},...,\mathrm{p}_N^{(r)},\tilde{\mathrm{p}}_1^{(\varphi)},...,\tilde{\mathrm{p}}_N^{(\varphi)}\right\}^T.$$

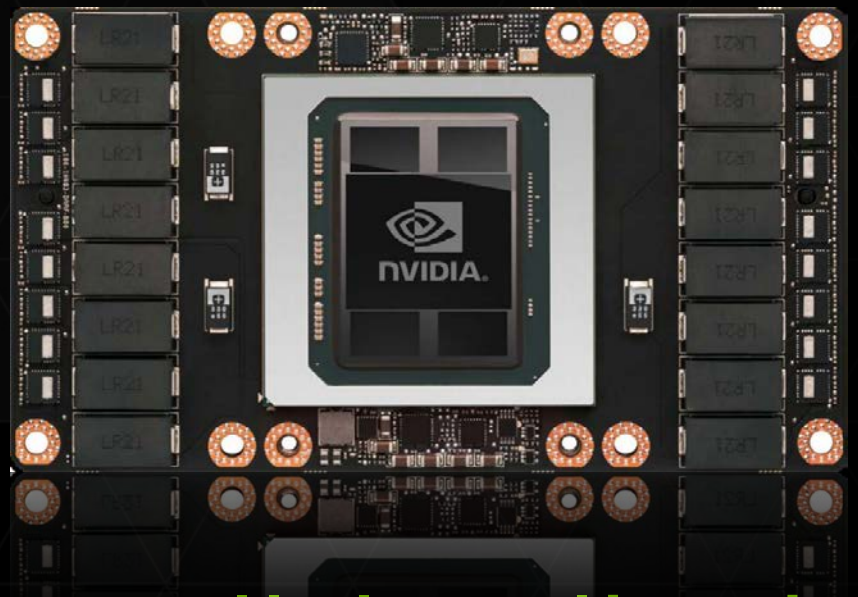
Motion equations $\boxed{\dot{\vec{\eta}}=\mathrm{G}_\gamma(t)\vec{\eta},}\ \mathrm{G}_\gamma(t)=\mathrm{G}\,\mathrm{E}(t),\ \mathrm{E}(t)\overset{\text{def}}{=}\begin{pmatrix}e^{2\gamma t}\,\mathrm{I}_{2N} & 0\\ 0 & e^{-2\gamma t}\,\mathrm{I}_{2N}\end{pmatrix},$

Solution $\boxed{\vec{\eta}(t)=e^{-\gamma t}\mathcal{M}\left[\mathcal{E}(t)\vec{C}_+ +\mathcal{E}(-t)\vec{C}_-\right],}$ *where* $\vec{C}_\pm\overset{\text{def}}{=}\begin{pmatrix}\vec{A}_\pm\\ \vec{B}_\pm\end{pmatrix},\ \mathcal{M}\overset{\text{def}}{=}\begin{pmatrix}\mathrm{M}' & 0\\ 0 & \mathrm{M}''\end{pmatrix},\ \mathcal{E}(t)\overset{\text{def}}{=}\begin{pmatrix}e^{ti\bar{\Omega}} & 0\\ 0 & e^{ti\bar{\Omega}}\end{pmatrix},$

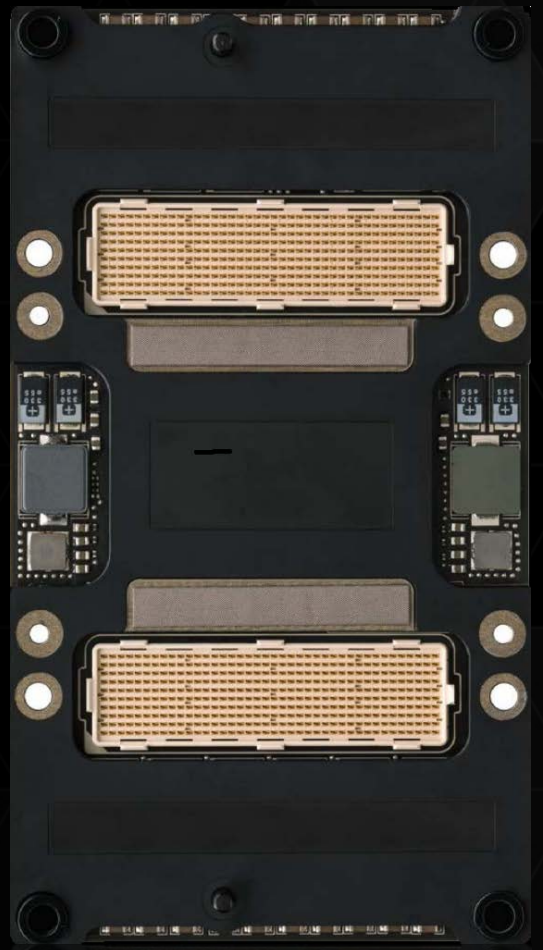
$$\vec{A}_\pm=\frac{1}{2}\mathrm{M}'^{-1}\left\{\vec{\eta}'(0)\pm\Gamma'^{-1}\left[\gamma\vec{\eta}'(0)+\mathrm{D}\vec{\eta}''(0)\right]\right\},\ \vec{B}_\pm=\frac{1}{2}\mathrm{M}''^{-1}\left\{\vec{\eta}''(0)\pm\Gamma''^{-1}\left[\gamma\vec{\eta}''(0)-\mathrm{K}\vec{\eta}'(0)\right]\right\},$$

$$\Gamma'\overset{\text{def}}{=}\mathrm{M}'i\bar{\Omega}\mathrm{M}'^{-1},\ \Gamma''\overset{\text{def}}{=}\mathrm{M}''i\bar{\Omega}\mathrm{M}''^{-1},\ \bar{\Omega}=\mathrm{diag}\left(\bar{\omega}_1,...,\bar{\omega}_{2N}\right),\ \bar{\omega}_k=\sqrt{\omega_k^2-\gamma^2},\ \mathcal{M}\mathcal{E}(\pm t)\mathcal{M}^{-1}=e^{\pm t\mathcal{G}},$$

$$\Omega^2\overset{\text{def}}{=}\mathrm{M}'^{-1}(\mathrm{D}\,\mathrm{K})\mathrm{M}'=\mathrm{M}''^{-1}(\mathrm{K}\,\mathrm{D})\mathrm{M}''=\mathrm{diag}\left(\omega_1^2,...,\omega_{2N}^2\right).$$



Parallel realization by GPU

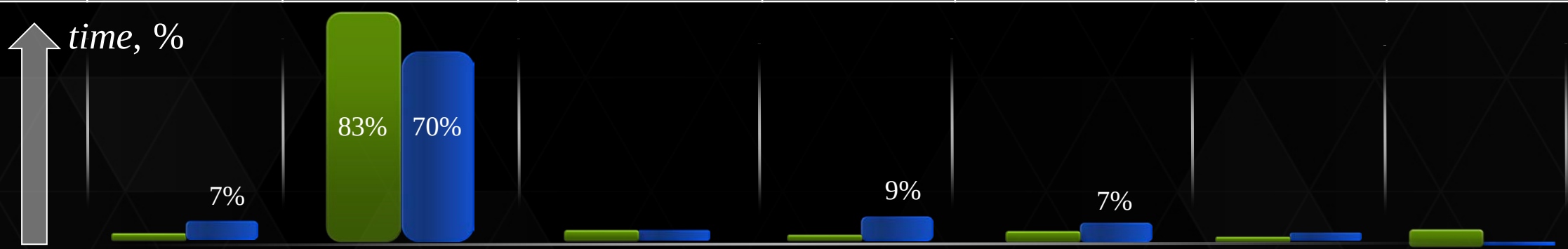


LIBRARIES

Google Colab: NVIDIA A100 40Gb CUDA 12.8

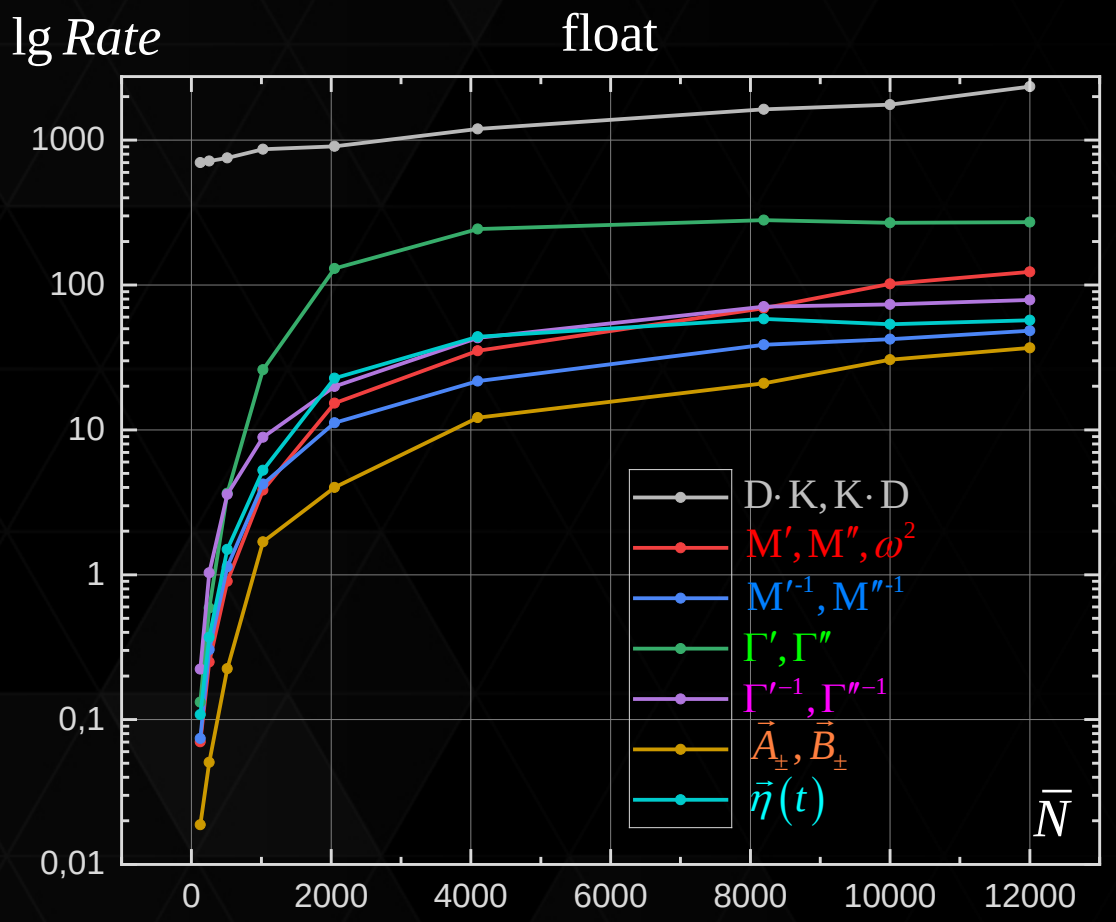
Google Colab: Intel Xeon Skylake-SP CPU 2GHz Intel MKL 2025.0.0

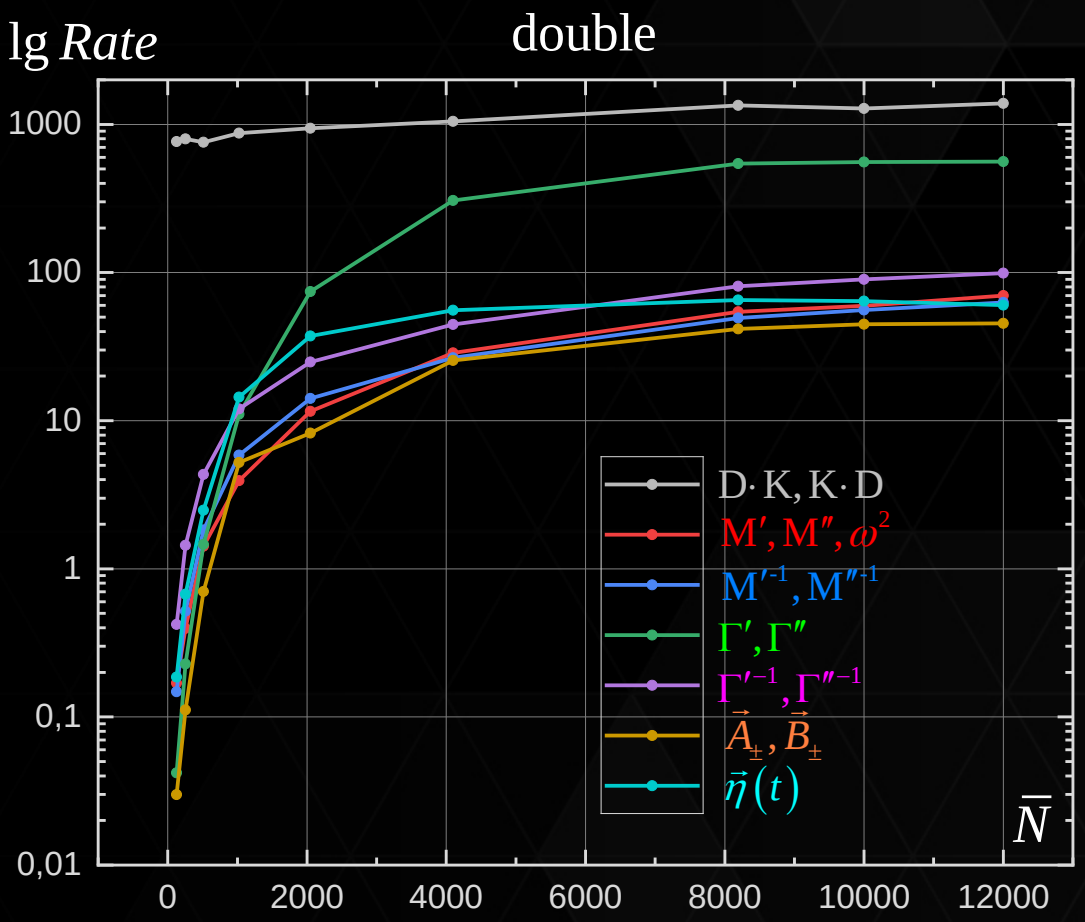
Block	$D \cdot K, K \cdot D$	M', M'', ω^2	M'^{-1}, M''^{-1}	Γ', Γ''	$\Gamma'^{-1}, \Gamma''^{-1}$	$\vec{A}_{\pm}, \vec{B}_{\pm}$	$\vec{\eta}(t)$
CPU	cblas_sscal	LAPACKE_sgeev	LAPACKE_sgetrf LAPACKE_sgetrs	cblas_cgemm	LAPACKE_sgetrf LAPACKE_sgetrs	cblas_caxpy cblas_cgemm cblas_cgemv	cblas_cgemv
GPU	cublasSdgmm	cusolverDnXgeev	cusolverDnSgetrf cusolverDnSgetrs	cublasCgemm	cusolverDnSgetrf cusolverDnSgetrs	cublasCaxpy cublasCscal cublasCgemv	cublasCaxpy cublasCscal cublasCgemv



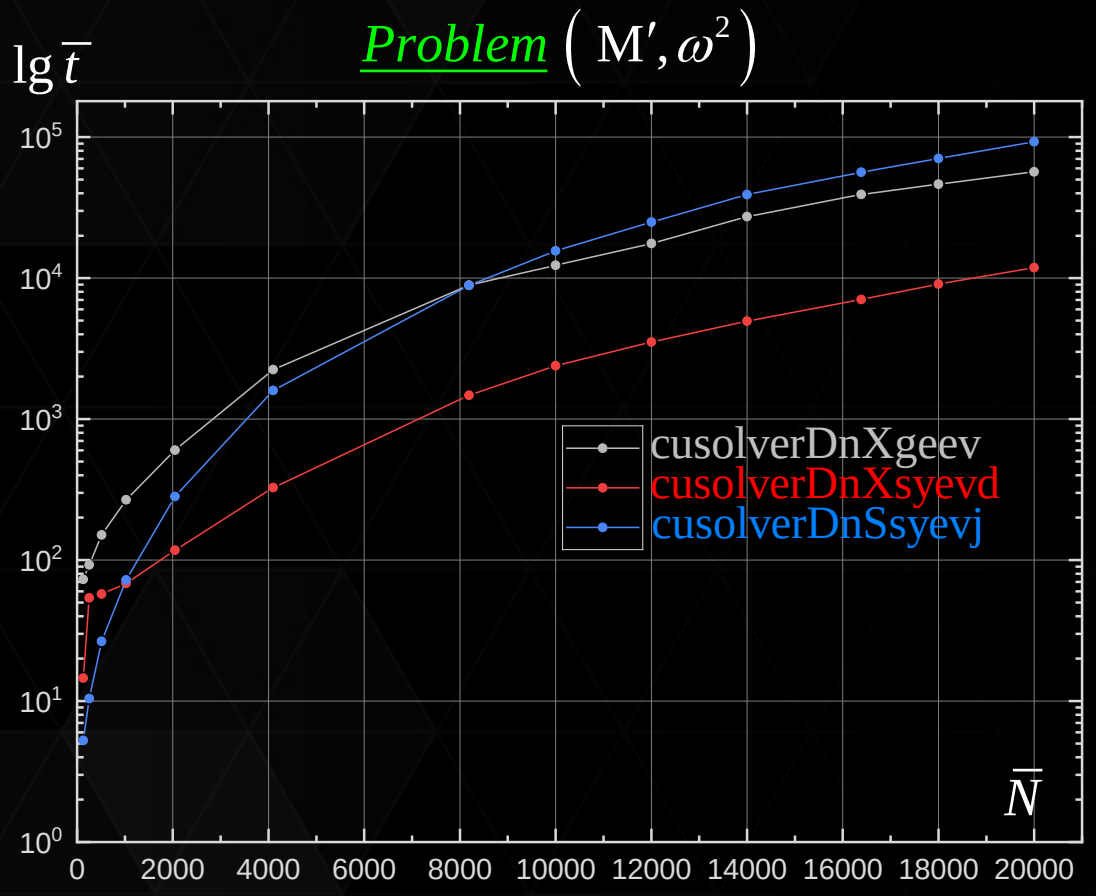
CPU VS GPU

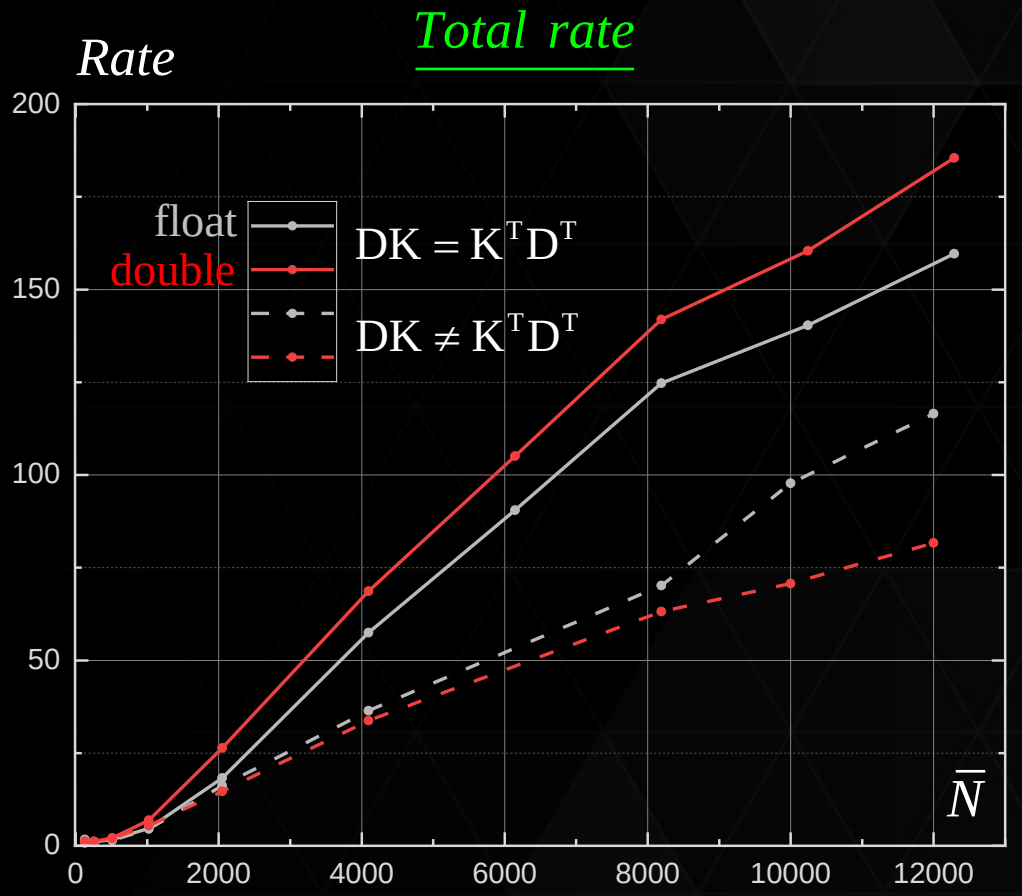
Rate = time_CPU / time_GPU



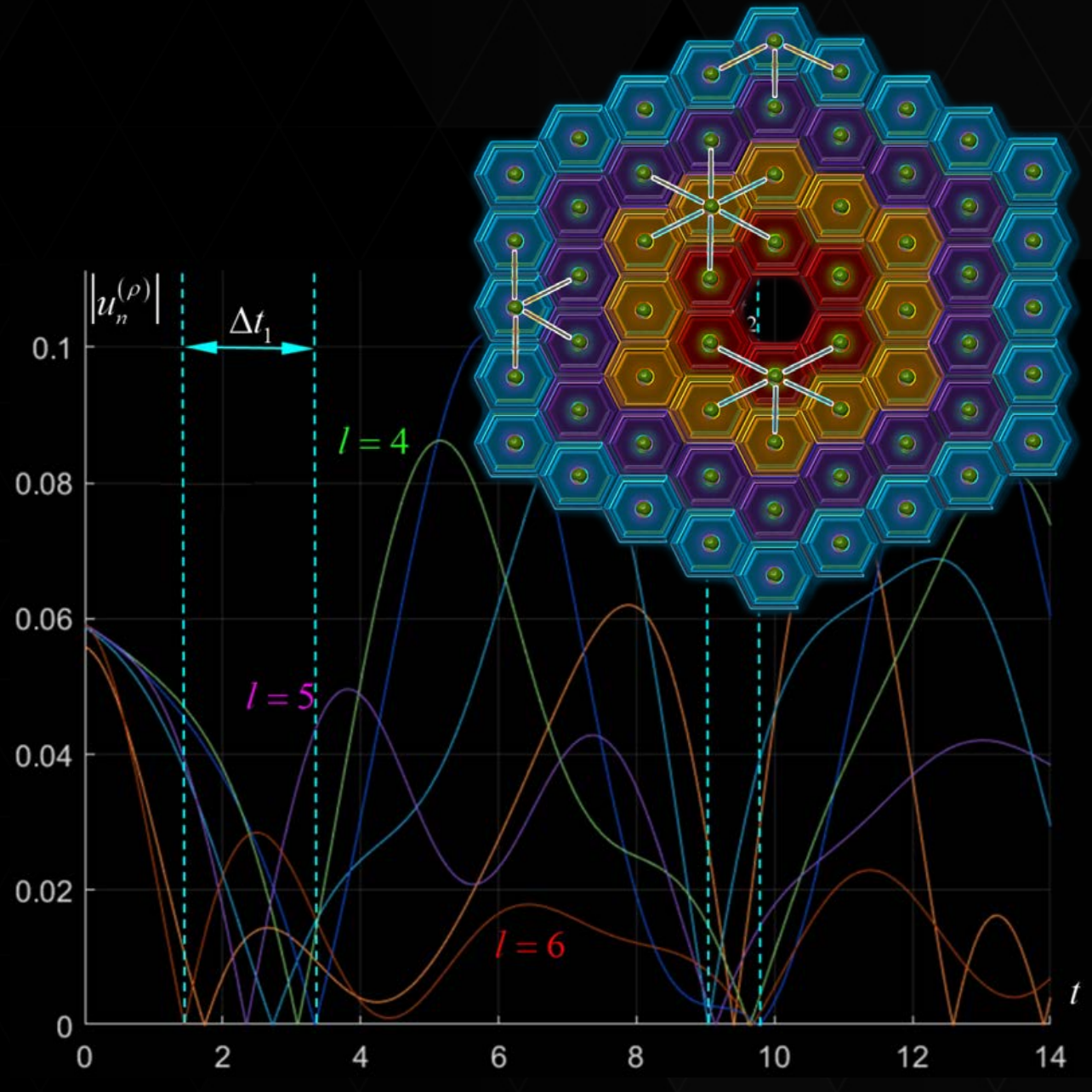


TOTAL RATE

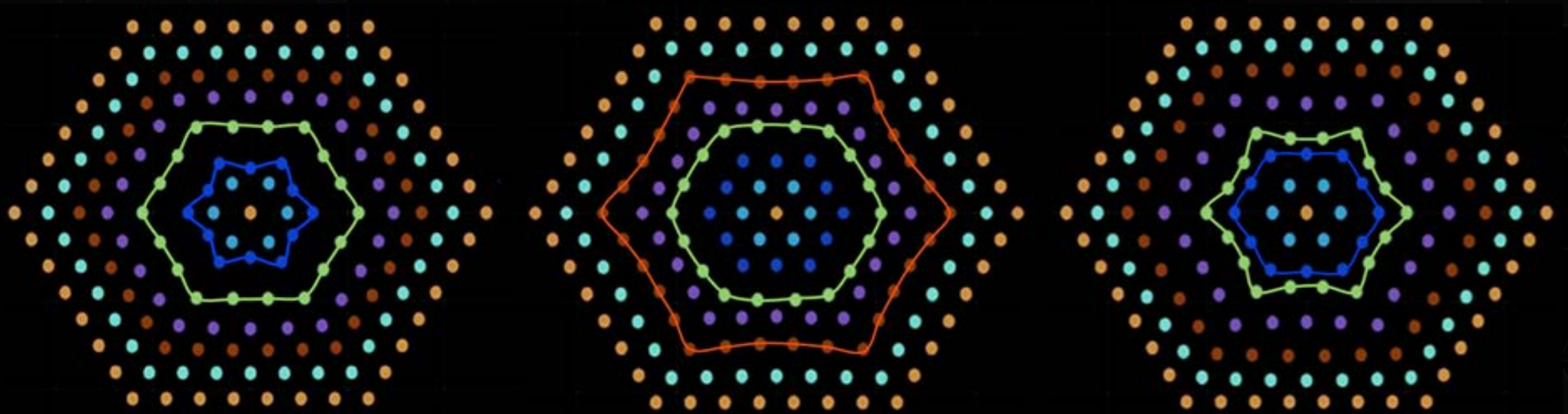




Results



SYMMETRIC CONFIGURATIONS OF RADIAL DISPLACEMENTS OF THE RODS

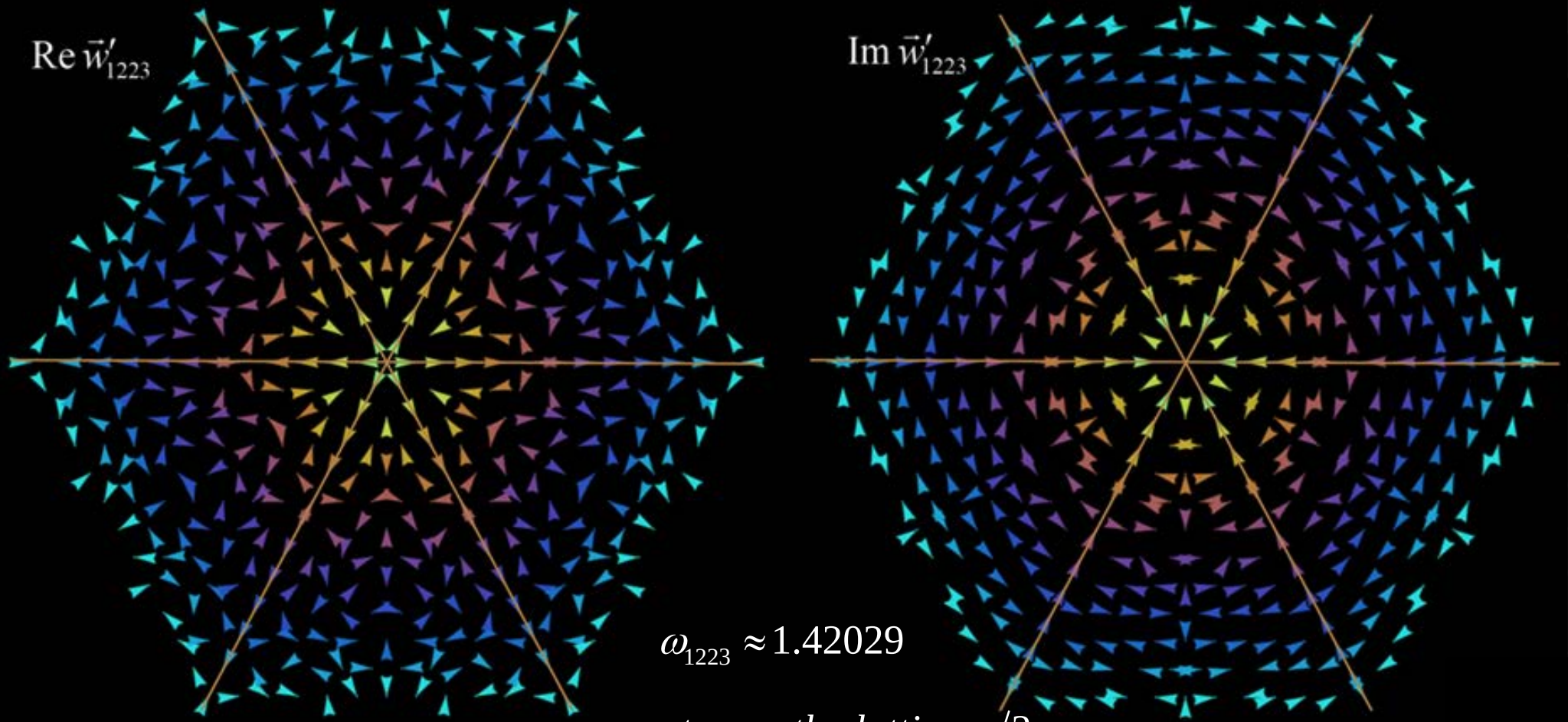


Initial conditions $u_n^{(\rho)}\Big|_{t=0} = \left(\vec{u}_n, \vec{e}_\rho\right) = 0,\ u_n^{(\varphi)}\Big|_{t=0} = \left(\vec{u}_n, \vec{e}_\varphi\right) = 0,\ n \in N,$

$$v_n^{(\rho)}\Big|_{t=0} = \left(\vec{v}_n, \vec{e}_\rho\right) = \begin{cases} v_0, & n \in \Omega^1 \\ 0, & n \in \Omega^l, l = 2...L \end{cases}, \qquad v_n^{(\varphi)}\Big|_{t=0} = \left(\vec{v}_n, \vec{e}_\varphi\right) = 0.$$

COMPONENTS OF EIGENVECTORS

Coordinate and momentum representations for the system of 468 elements

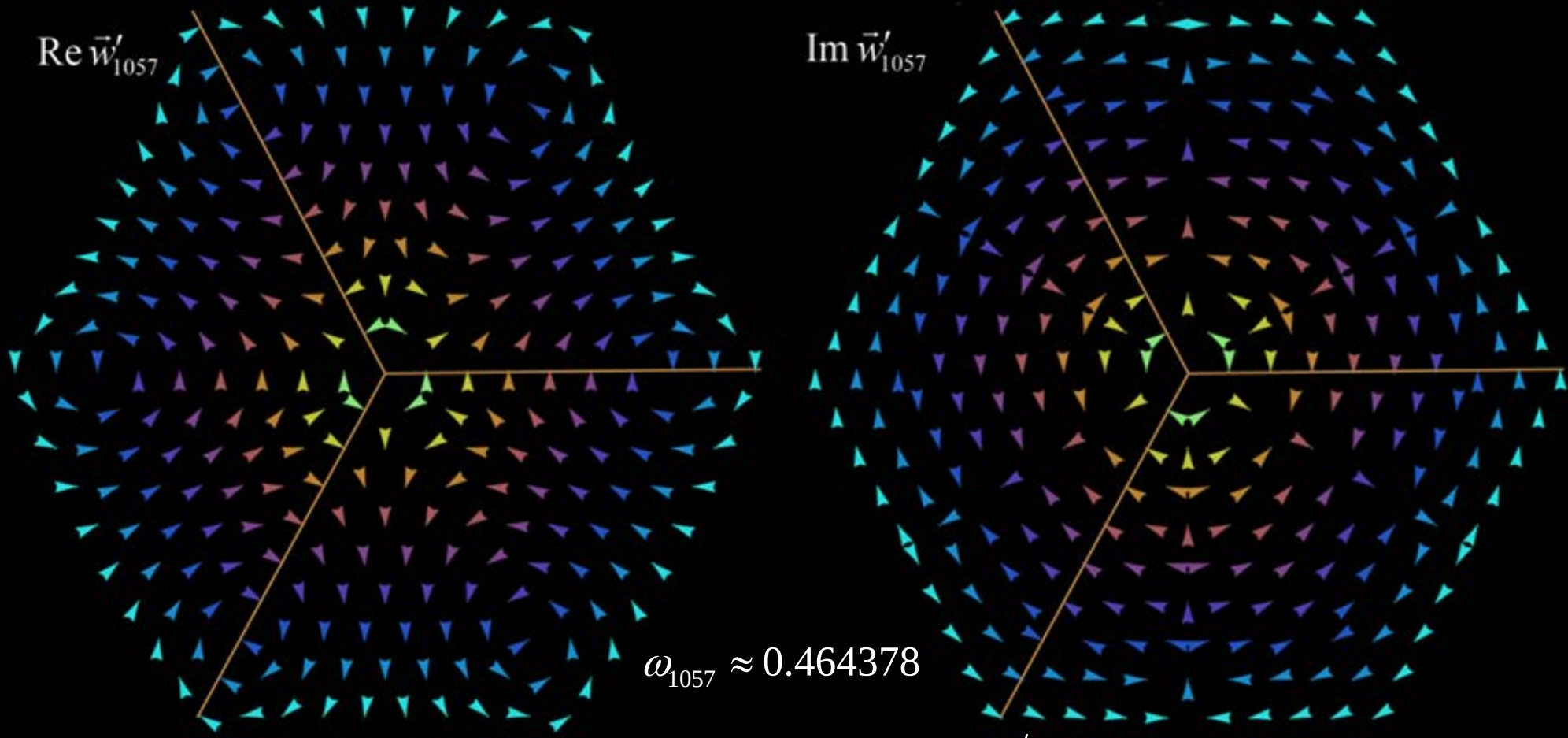


$\omega_{1223} \approx 1.42029$

symmetry on the lattice $\pi/3$

COMPONENTS OF EIGENVECTORS

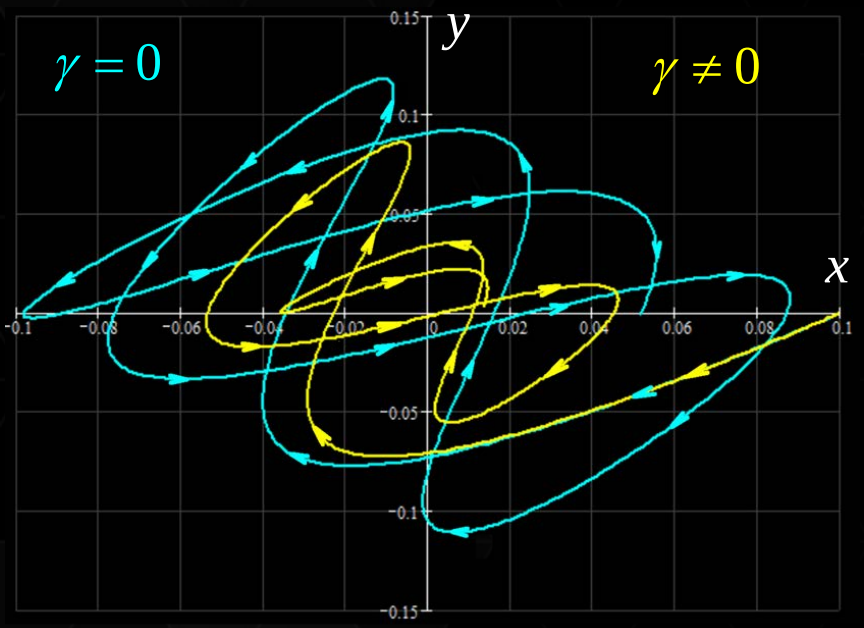
Coordinate and momentum representations for the system of 468 elements



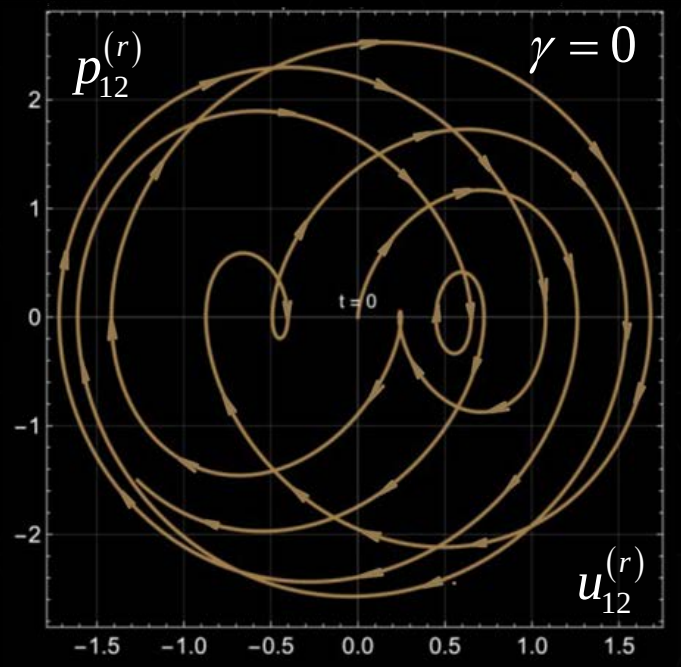
$\omega_{1057} \approx 0.464378$

symmetry on the lattice $2\pi/3$

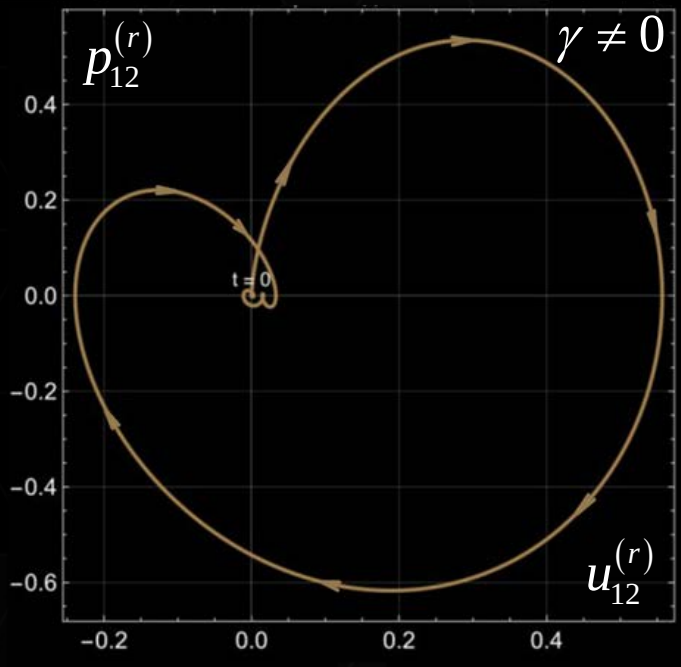
DISSIPATIVE SYSTEM



"*center*"



"*focus*"



CONCLUSION

- An important advantage of the proposed approach is the speed of numerically finding the phase trajectories of the system.
- Note that in practice, initial state of the system $\boldsymbol{\eta_0} = \boldsymbol{\eta}(0)$ is never exactly known. In reality, there exists multidimensional (4N) phase region V_0 of admissible initial parameters of the system. Thus, it is necessary to map initial region V_0 into region V_t, corresponding to moment of time t. Such a procedure requires multiple calculations for the set of initial states of the system $\boldsymbol{\eta_0} \in V_0$. Knowing region V_t, the elements of which are $\boldsymbol{\eta}(t)$, it is possible to make an estimate of the stability parameters of the reactor.