Simulation of Nonlinear Dynamics in Large Neuronal Networks Using ARC Middleware

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Ukrainian National Grid (UNG)

Since 2006

Initiatitors:

BITP, KNU

Now

~30 clusters

~3500 CPUs

Grid Monitor - Mozilla Firefox

www.nordugrid.org/monitor/loadmon.php?display=vo=Uk

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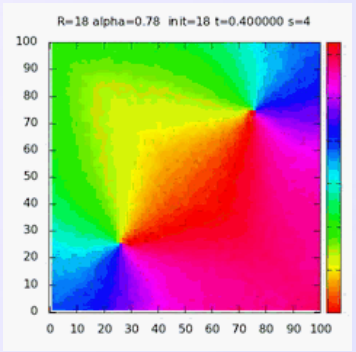
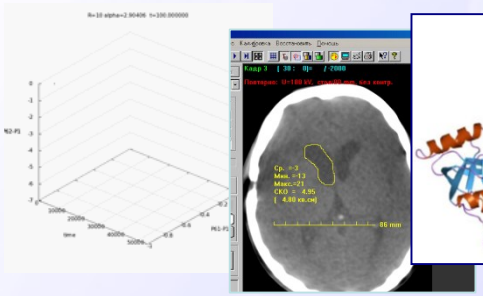
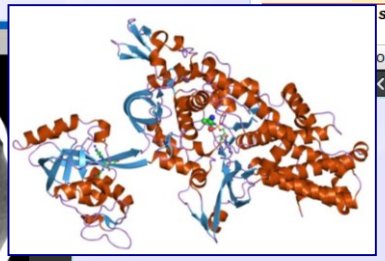
Processes: Grid Local

Country	Site	CPUs	Load (processes: Grid+local)	Queueing
	Chernihiv NTU Cluster	1	0+0	0+0
	CHIMERA	168	0+3	1975+0
	IAPMM Cluster	36	0+1	1+0
	ICMP Cluster	320	60+47	0+0
	ICYB SCIT-3	1480	0+288	0+0
	IEP Cluster	52	0+0 (queue inactive)	0+0
	IFBG Cluster	64	0+0	0+0
	ILTPE ARC UA	80	10+0	0+0
	IMATH Cluster	16	0+2	1+0
	IMBG ARC	360	0+288 (queue inactive)	103+0
	IMMSP Cluster	40	0+0	5+0
	IMP ARC	76	0+13	0+0
Ukraine	INPARCOM Cluster	8	0+0	0+0
	INPARCOM GPU Cluster	8	0+0	0+0
	IPM Cluster	40	0+0	0+0
	IPMS Cluster	32	0+16	0+0
	IRE Cluster	80	0+76	0+2
	ISMA cluster	264	49+77	0+0
	ISOFTS Cluster	0		0+0
	KIPT IPP	48	0+0	0+0
	KNU ARC	80	51+1	4+2
	KPI training cluster	24	0+0	0+0
	LNU Training Cluster	32	0+0 (queue inactive)	0+0
	MAO Cluster	88	23+36	28+0
	MHI Cluster	136	0+0	0+0
	PIMEE ARC	24	0+0	4+0
	sites	3557	193 + 848	2121 + 4

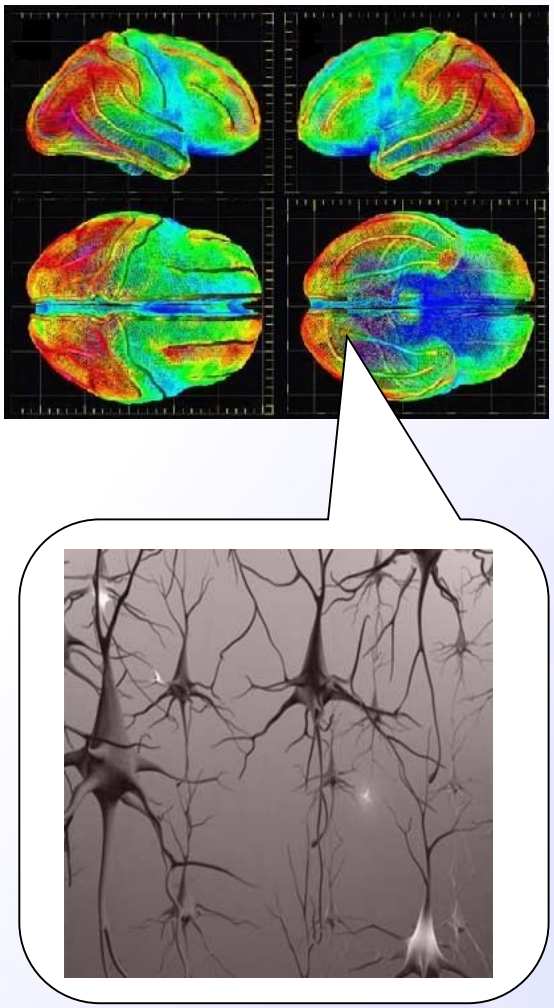
org/monitor/jobstat.php?host=...rkov.ua&port=2135







Simulation of neurosystems



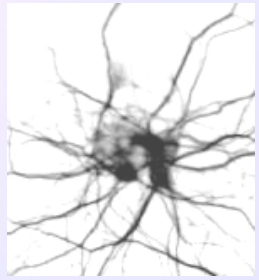
- **Nervous system functions**
  - **Cognition**
  - **Memory**
  - …
- **Neuronal pathologies**
  - **Parkinson disease**
  - **Epilepsy**
- **Complicated mathematical models**
  - **1 neuron 1-15 nonlinear ODE**
  - **10^2-10^8 coupled neurons**
  - **Any links topology**
  - **Large parameters number 10^0-10^1**
  - **1 trajectory 10^{11}-10^{14} operations**
  - **1 trajectory 0.1-10 Гбайт даних**
  - **1 task 10^1-10^3 trajectories**
- **Very resource consuming**
  - **Grid is solution**
  - **VO networkdynamics in UNG**

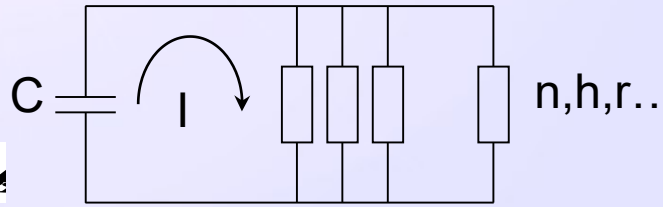
Model of Parkinson disease: Rubin-Terman 2007

Subthalamic Nucleus (STN) and Globus Pallidus External (GPe)

Neuron is described by **6** dynamic variables

- V – membrane potential
- n – conductivity of K – channels
- h – conductivity of Na-channels
- r – conductivity of low-threshold Ca-channels
- [Ca] – intercellular concentration of Ca-ions
- s – synaptic conductivity from neuron
- Non-linear functions





6 nonlinear Hodgkin-Huxley ordinary differential equations

$$C\frac{dV}{dt} = -I_L(V) - I_K(V,n) - I_{Na}(V,h) - I_T(V,r) - I_{Ca}(V) - I_{AHP}(V,[Ca]) - I_s(V,\sum_j s_j) - I_{app}(\mathrm{t})$$

$$\frac{dn}{dt} = f_n(V,n);\ \frac{dh}{dt} = f_h(V,h);\ \frac{dr}{dt} = f_r(V,r);\ \frac{d[Ca]}{dt} = f_{Ca}(I_{Ca},I_T,[Ca]);\ \frac{ds}{dt} = f_s(V,s)$$

Rubin-Terman model

Model of a single STN neuron

$$
\begin{aligned}
C_m v' &= -g_{\mathrm{L}}\left(v-v_{\mathrm{L}}\right)-g_{\mathrm{K}} n^4\left(v-v_{\mathrm{K}}\right)-g_{\mathrm{Na}} m_\infty^3(v) h\left(v-v_{\mathrm{Na}}\right)-g_{\mathrm{T}} a_\infty^3(v) b_\infty^2(r)\times \\
&\quad \times\left(v-v_{\mathrm{Ca}}\right)-g_{\mathrm{Ca}} s_\infty^2(v)\left(v-v_{\mathrm{Ca}}\right)-g_{\mathrm{AHP}}\left(v-v_{\mathrm{K}}\right)\frac{[\mathrm{Ca}]}{[\mathrm{Ca}]+k_1}-I_{\mathrm{GPe}\to\mathrm{STN}}+ \\
&\quad +I_{\mathrm{DBS}}, \\
n' &= \phi_n\left(\frac{1}{1+\exp[-(v-\theta_n)/\sigma_n]}-n\right)/\tau_n(v), \\
h' &= \phi_h\left(\frac{1}{1+\exp[-(v-\theta_h)/\sigma_h]}-n\right)/\tau_h(v), \\
r' &= \phi_r\left(\frac{1}{1+\exp[-(v-\theta_r)/\sigma_r]}-n\right)/\tau_r(v), \\
[\mathrm{Ca}]' &= \epsilon\left(-g_{\mathrm{Ca}} s_\infty^2(v)\left(v-v_{\mathrm{Ca}}\right)-g_{\mathrm{T}} a_\infty^3(v) b_\infty^2(r)\left(v-v_{\mathrm{Ca}}\right)-k_{\mathrm{Ca}}[\mathrm{Ca}]\right), \\
s' &= \alpha\frac{1}{1+\exp\left[-\left(v-\theta_g-\theta_g^{\mathrm{H}}\right)/\sigma_g^{\mathrm{H}}\right]}(1-s)-\beta s,
\end{aligned}
$$

where v is the membrane potential, I_{DBS} – the applied stimulation current, $I_{\mathrm{GPe}\to\mathrm{STN}}$ – the influence of the GPe onto STN. The interaction between the neurons can be written as:

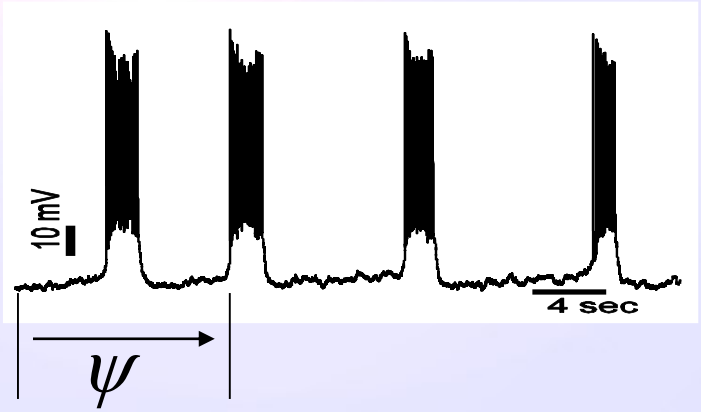
$$
\begin{aligned}
I_{\mathrm{GPe}\to\mathrm{STN}} &= g_{\mathrm{G}\to\mathrm{S}}(v-v_{\mathrm{G}\to\mathrm{S}})\sum_{j \text{ in GPe}} s_j, \\
I_{\mathrm{DBS}} &= i_D H\left(\sin\left(2\pi t/\rho_D\right)\right)\times\left[1-H\left(2\pi\left(t+\sigma_D\right)/\rho_D\right)\right].
\end{aligned}
$$

Phenomenological model Kuramoto-Sakaguchi

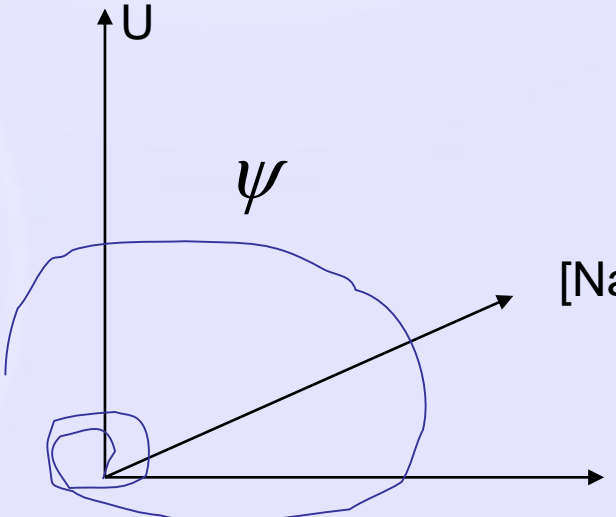
Single variable **phase** instead of many dynamical variables
Phase – position of system state in phase space
Describes synchronization in any system
Equations are very simple

$$\dot{\psi}_i = \frac{1}{2R}\sum_{|j|\le R}\sin\left(\psi_j - \psi_i - \alpha\right), \quad i = 1,\ldots,N.$$

R- number of links
A – degree of excitation/inhibition

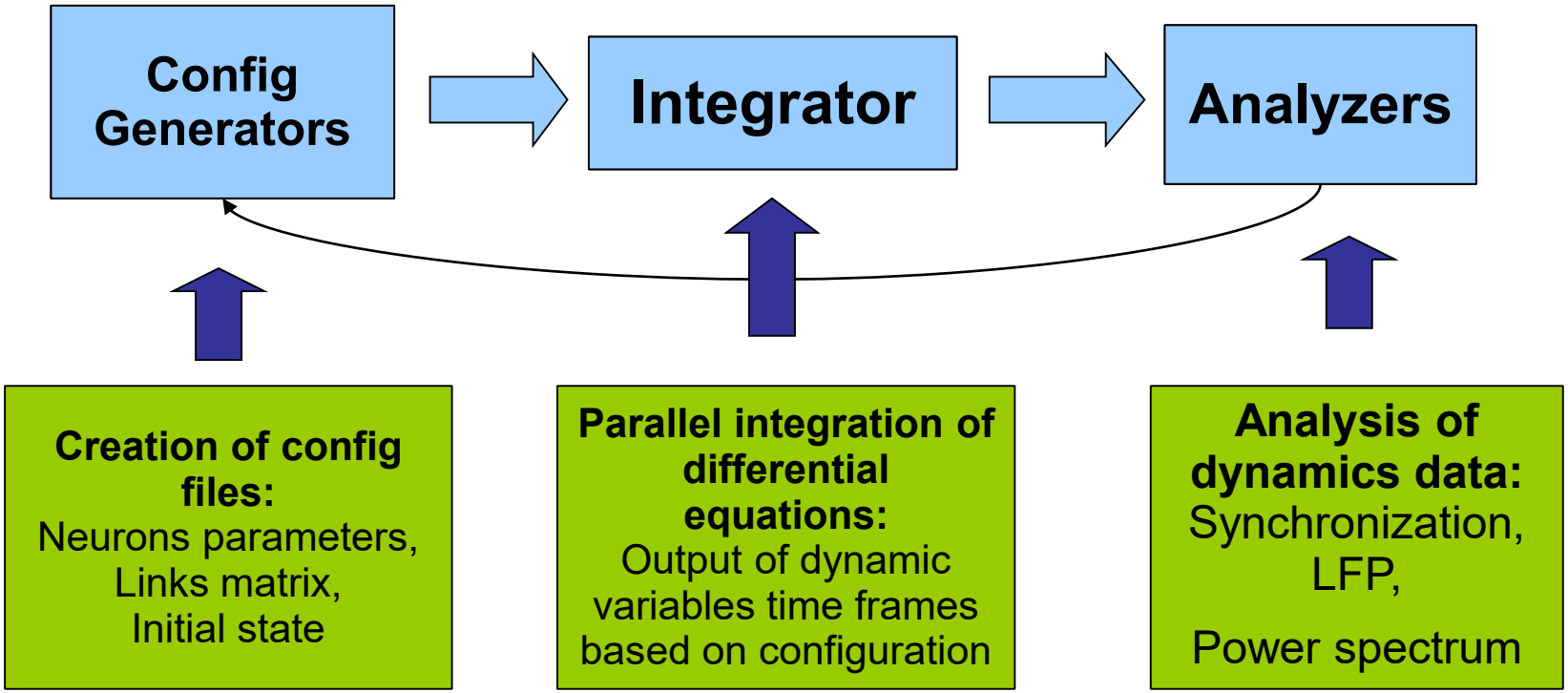


Chimera state
Stationary state with sync and chaos

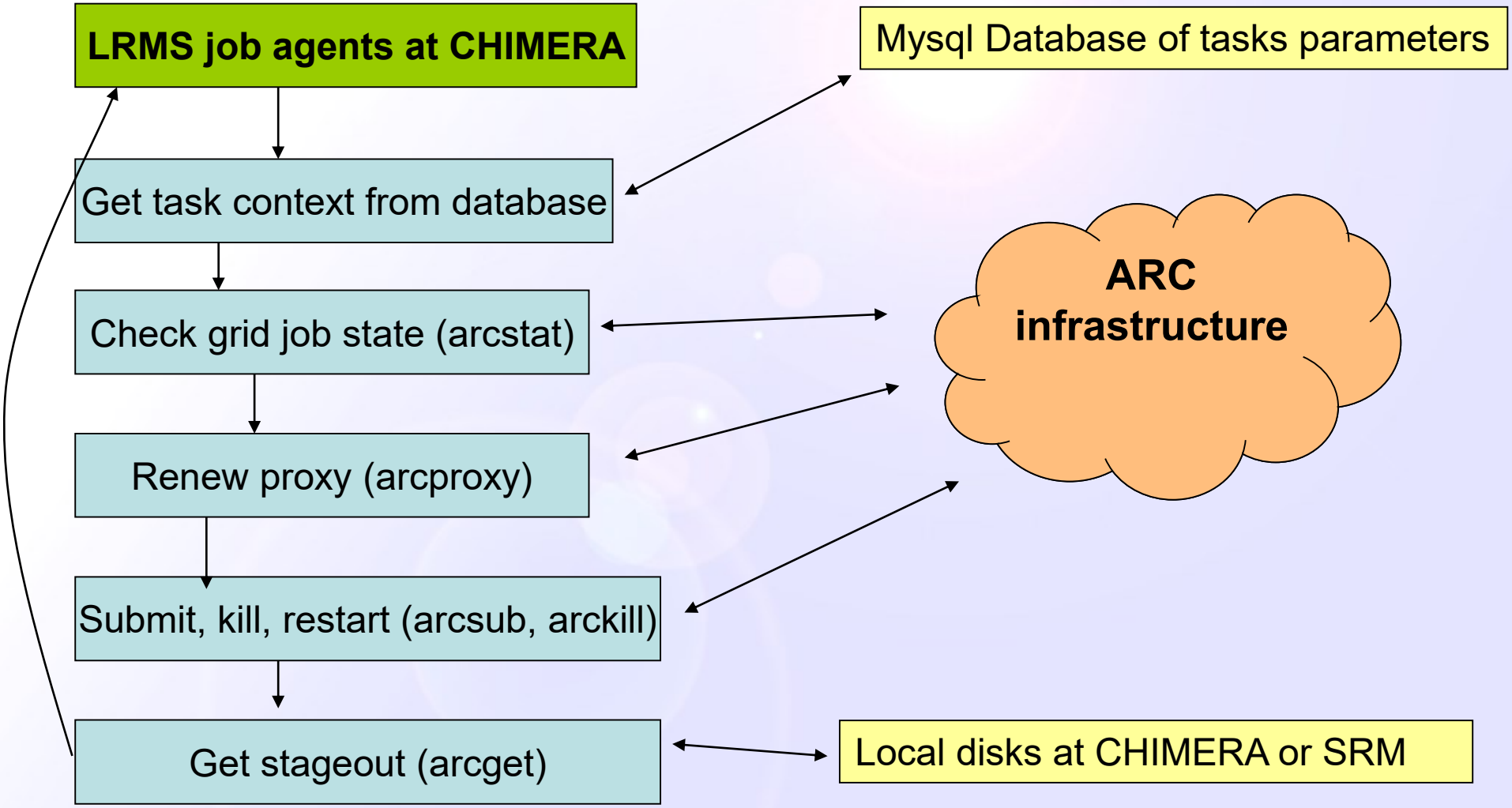


Simulation Software

- Parallel DOPRI, BDF, IE integrator
  - C++
  - OpenMP
  - MPI
  - SUNDIALS
  - Easy new model integration
  - Links Topology compression



Grid jobs driver



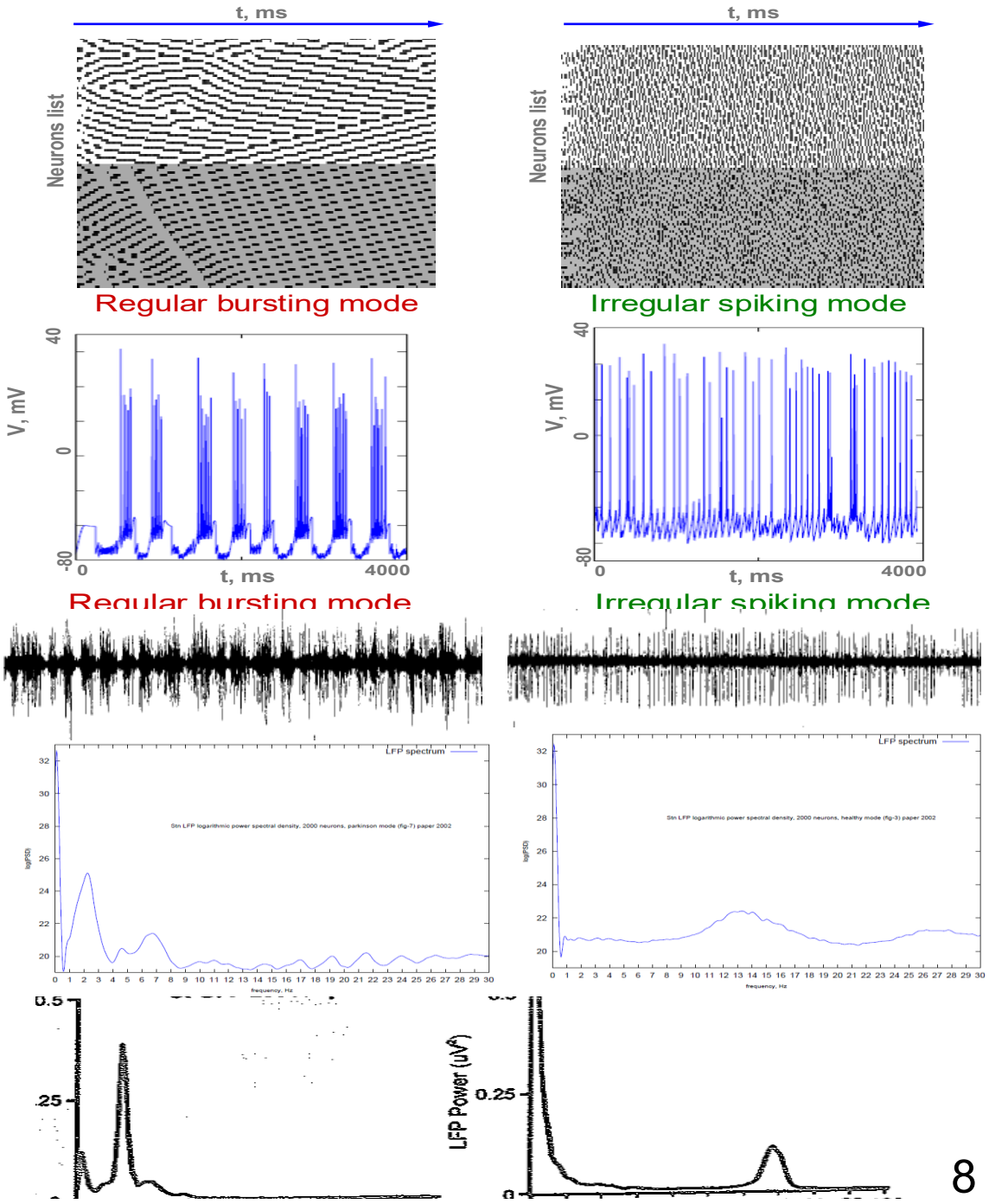
Simulation results for Parkinson disease

640 trajectories
10 sec dynamics
2000 neurons

Two modes

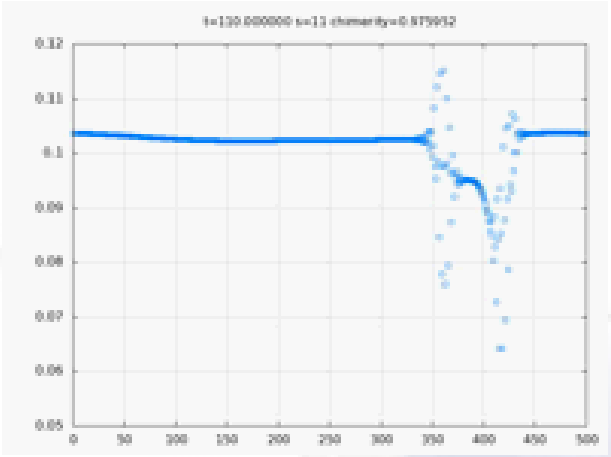
- **Regular bursting**
- **Irregular spiking**

- **Modes determined by links**



1-d chimera 10^3 neurons

Dynamics



Different chimera types

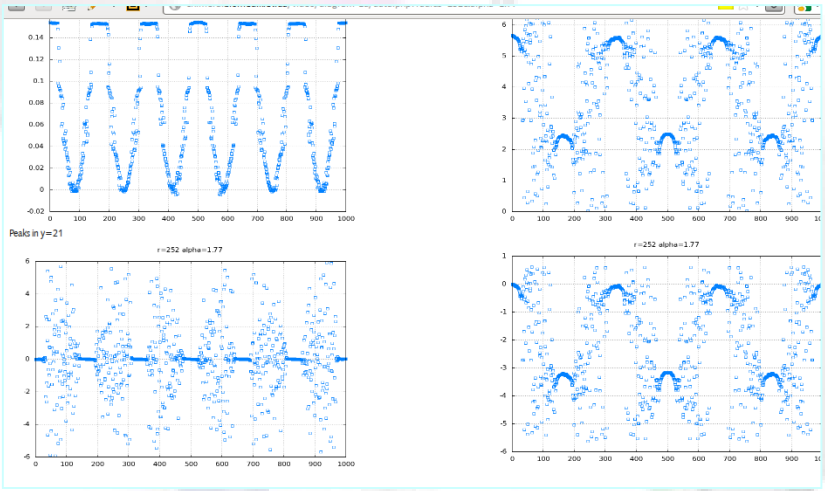
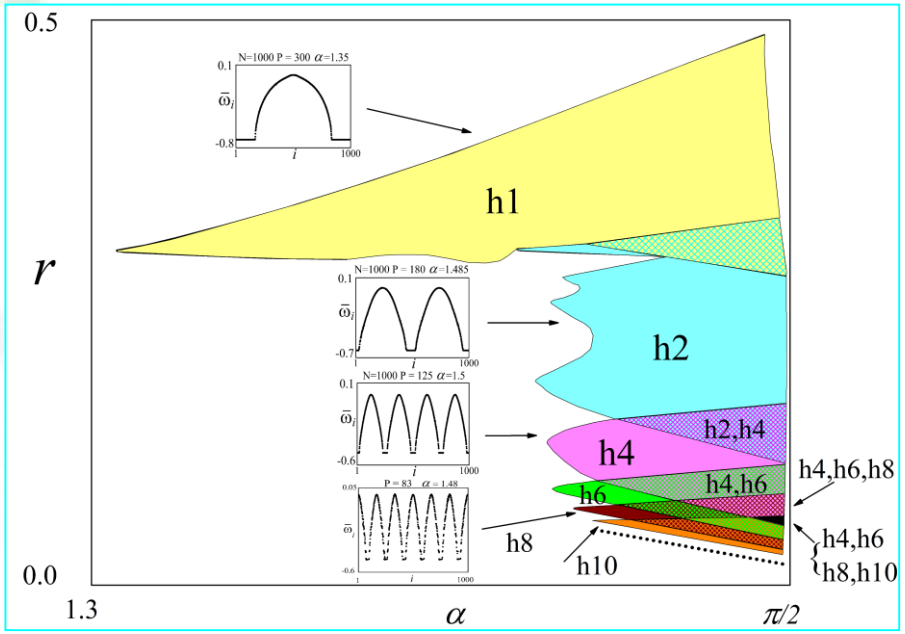
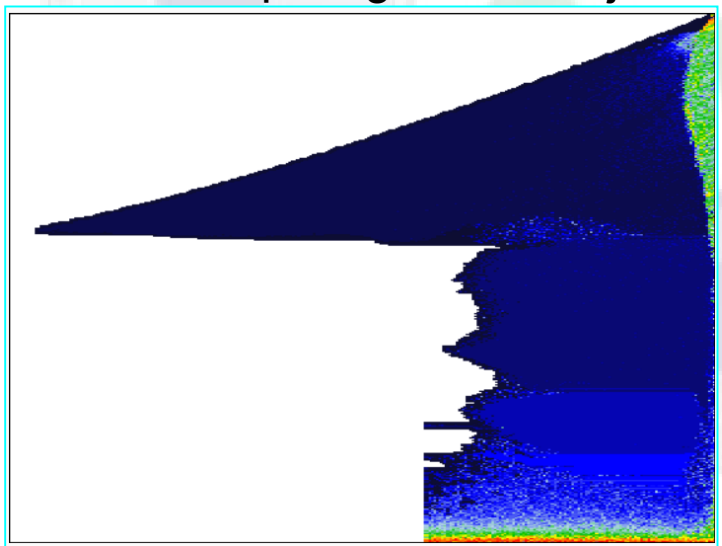


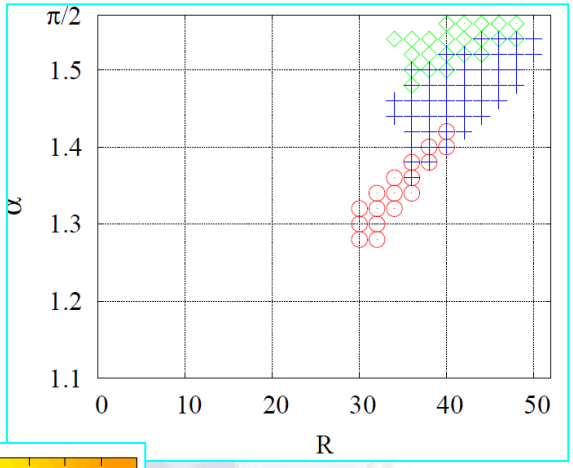
Diagram of different chimera states



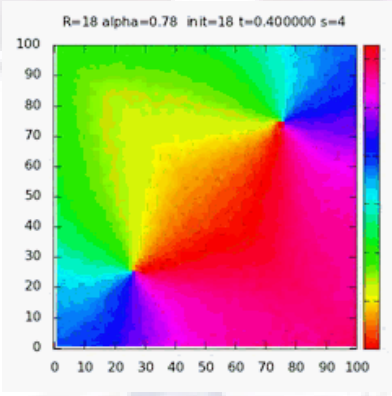
Grid computing 75000 trajectories

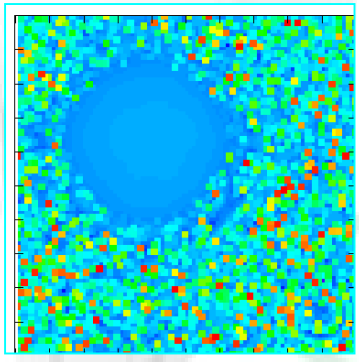


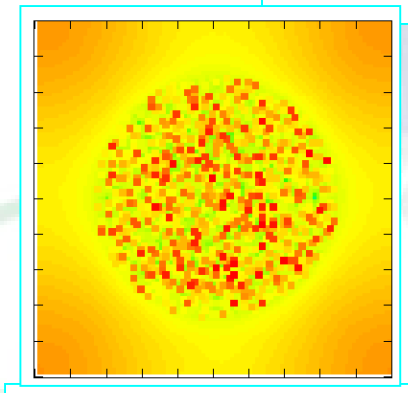
2d chimera 10^5 neurons ~1000 trajectories



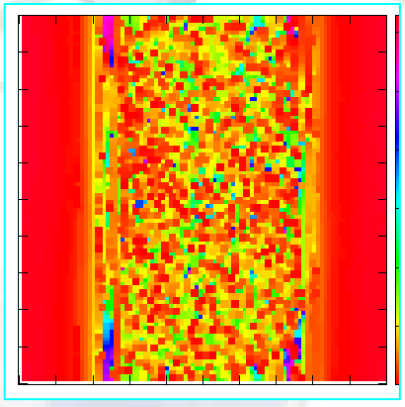
"Dying" of chimera

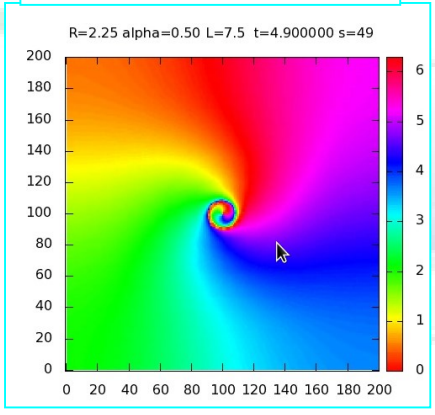


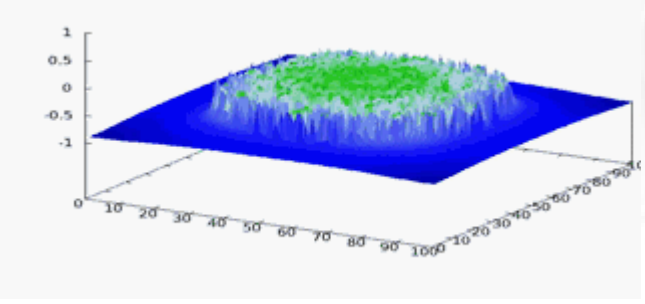




Living "chimera"



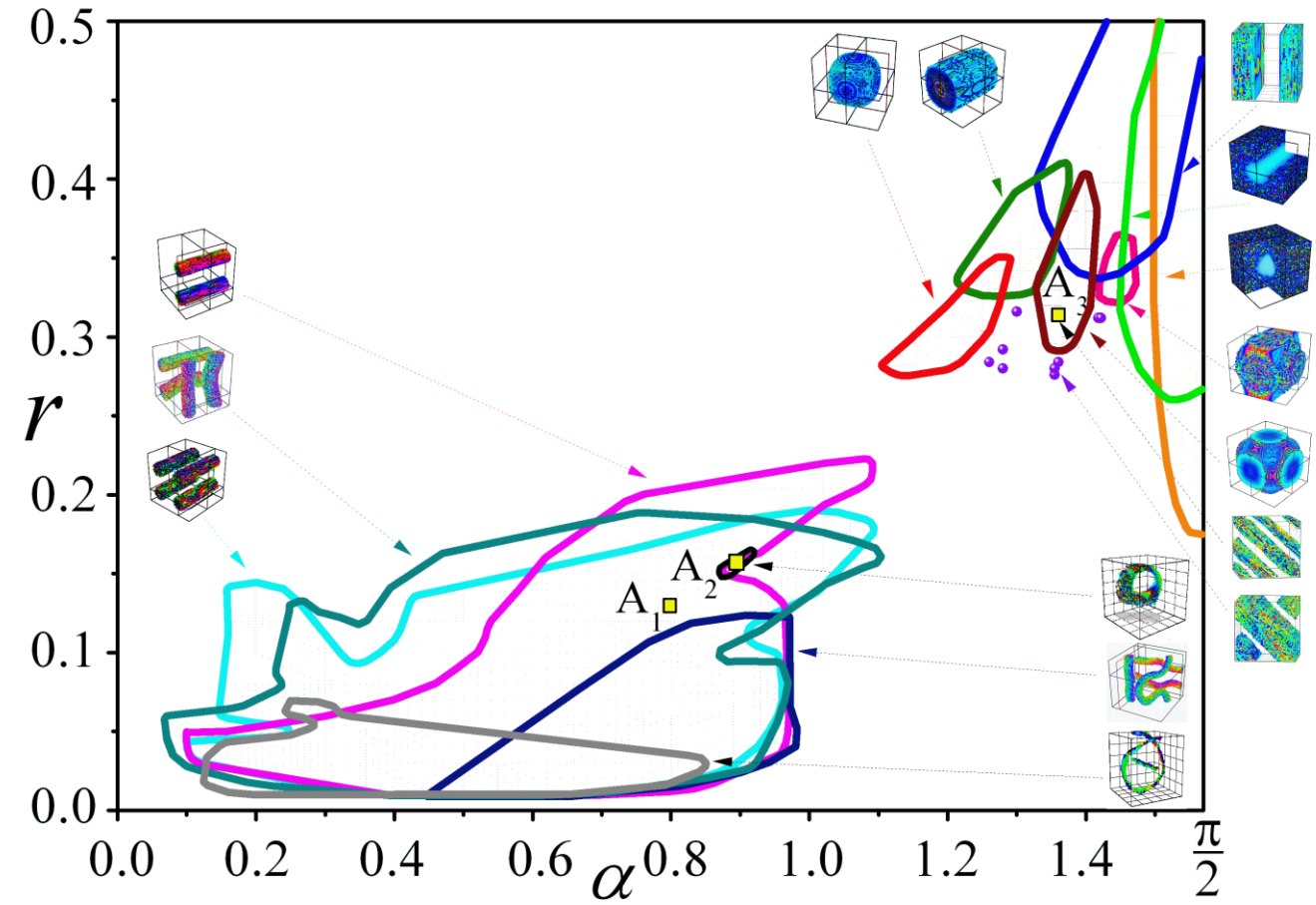


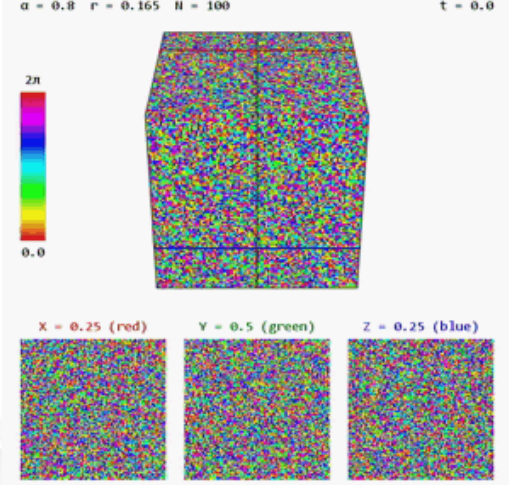


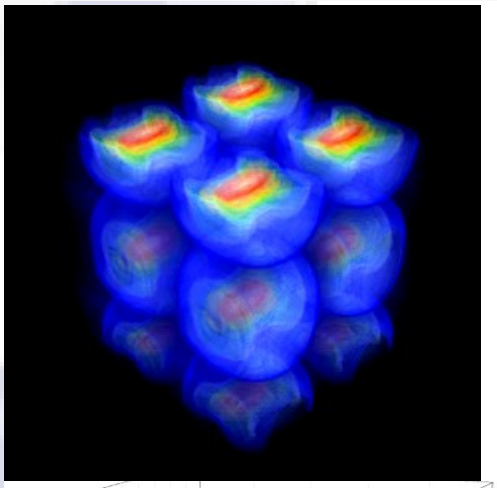
Types of chimera

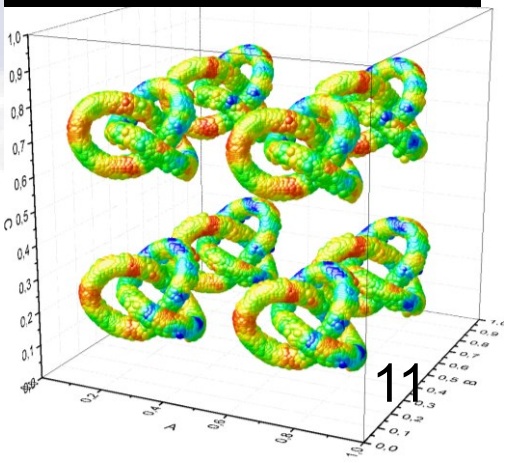
3d chimera 10^8 neurons

Diagram of chimera states





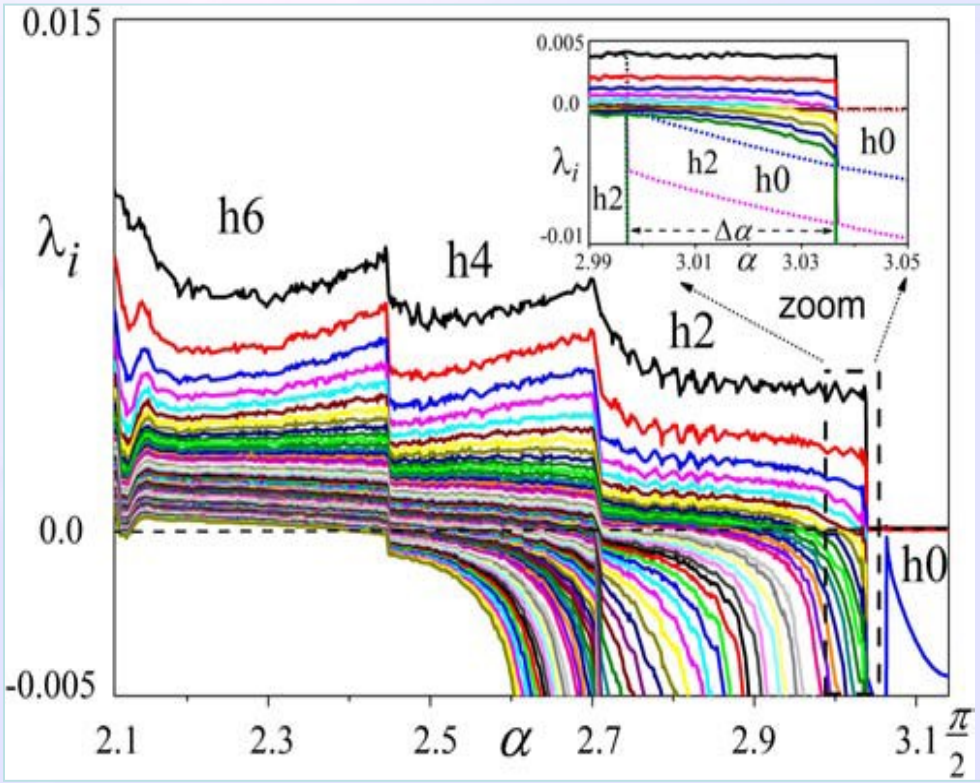




Lyapunov exponents computing

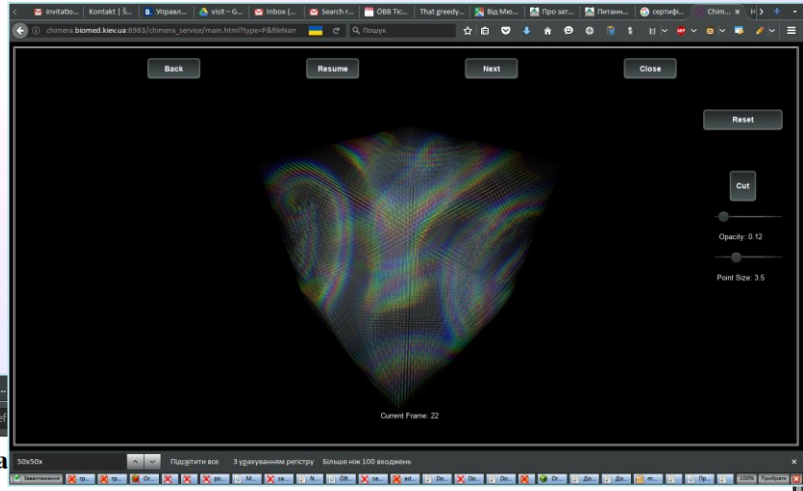
$$\frac{d\vec{x}}{dt} = \vec{f}(\vec{x}, t); \qquad \vec{\lambda} = \frac{1}{T}\int_0 \log(eig(\frac{\partial \vec{f}(\vec{x}(t), t)}{\partial \vec{x}}$$

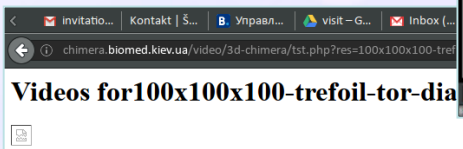
- N^3 operation per integration step
- 1-2 weeks on 8-16 CPUs
- 800 trajectories in Grid



Results, reports, visualization

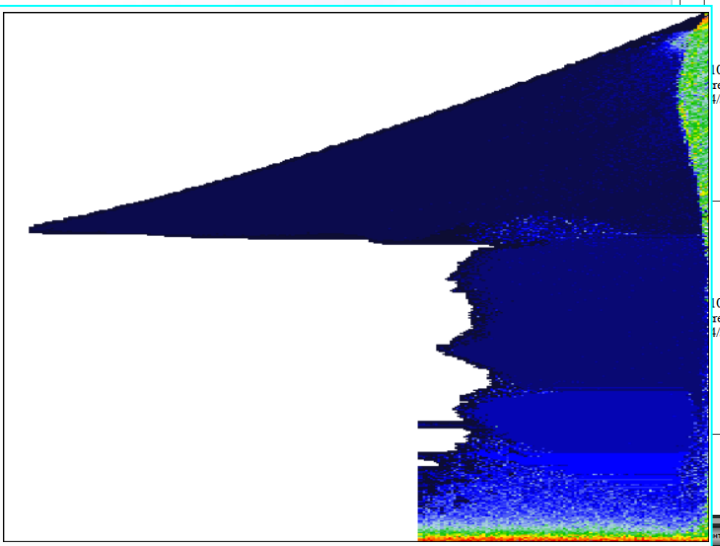
- Aggregate data
- Animations
- Interactive visualization





Videos for100x100x100-trefoil-tor-dia

#	Parameters	sections mean frequency	volume mean frequency	volume phase	Volum frequency	Config	
	100x100x100-refoil-tor-diag-l/alpha=.6285-r=4/	X Y Z 0 13 Unavailable Unavailable Unavailable 25 50 100 Unavailable Unavailable Unavailable	1 2 3	1 2 3 Experimental Interactive visualizer	1 2 3 Experimental Interactive visualizer	config (1954.06KB)	0.96616
	100x100x100-refoil-tor-diag-l/alpha=.6290-r=4/	X Y Z 0 13 Unavailable Unavailable Unavailable 25 50 100 Unavailable Unavailable Unavailable	1 2 3	1 2 3 Experimental Interactive visualizer	1 2 3 Experimental Interactive visualizer	config (1954.06KB)	0.96825
		X Y Z 0	1 2 3	1 2 3	1 2 3		



Selected publications

- Yuri Maistrenko, Oleksandr Sudakov, Oleksiy Osiv and Volodymyr Maistrenko//Chimera states in three dimensions. New J. Phys. 17 073037 doi:10.1088/1367-2630/17/7/073037
- O. E. Omel'chenko, M. Wolfrum, S. Yanchuk, Y. L. Maistrenko, O. Sudakov . Stationary patterns of coherence and incoherence in two-dimensional arrays of non-locally-coupled phase oscillators//Phys. Rev. E 85, 036210 (2012)
- Maistrenko, Y.L., Vasylenko, A., Sudakov, O., Levchenko, R., Maistrenko, V.L. Cascades of multiheaded chimera states for coupled phase oscillators // International Journal of Bifurcation and Chaos 24 (8), 1440014.
- Zynovyev, M., Svistunov, S., Sudakov, O., & Boyko, Y. “Ukrainian Grid infrastructure: practical experience,” 4-th International Workshop on Intelligent Data Acquisition and Advanced Computing Systems: Technology and Applications. Dortmund, Germany, September 6-8, 2007 pp. 237-240
- Y. O. Koval, H. O. Mendrul, A. O. Salnikov, I. A. Sliusar and O. O. Sudakov, "Interactive dynamical visualization of big data arrays in grid," Intelligent Data Acquisition and Advanced Computing Systems: Technology and Applications (IDAACS), 2015 IEEE 8th International Conference on, Warsaw, 2015, pp. 153-156.
- Salnikov, Andrii, Oleksandr Sudakov, Roman Levchenko, Ievgen Sliusar, & Anton Savchenko. "INTERACTIVE ENVIRONMENT FOR MASSIVE NEUROSCIENCE SIMULATIONS IN GRID." International Journal of Computing, 11.4 (2012): 367-374.
- Yuriy Maistrenko, Oleksandr Sudakov, Oleksiy Osiv, Volodymyr Maistrenko. “Chimera States in Three-Dimensions,” New Journal of Physics, vol. 17, 073037 (2015)

Conclusions

- ARC Grid provides unique facilities for simulations of large neuronal networks
- Some conditions for pathological synchronizations during Parkison disease and epilepsy were discovered using grid
- New types of chimera states in large coupled networks were discovered using grid
- Collaboration with Bogomolets Institute for Physiology NASU and other institutions are in progress in the field of neuronal networks modeling

Acknowledgements

- Resources of Ukrainian grid infrastructure were used for simulations

- Software development and testing was performed at computing clusters of Information and computer center National Taras Shevchenko University of Kyiv and National Scientific Center for medical and biotechnical problems NAS of Ukraine

- Some presented results were obtained in collaboration with Bogomolets Institute for Physiology NAS of Ukraine, Juelich Research Center Germany, Weierstrass Institute for Applied Analysis and Stochastics Germany

Thank you for attention!