



Molecular dynamics simulations in the MolDynGrid Virtual Laboratory by means of "ARC between Grid and Cloud"

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NORDUGRID Grid Solution for Wide Area Computing and Data Handling

MolDynGrid Virtual Laboratory

MolDynCrild Viriual Laboratory

Has been established in 2008 for interdisciplinary studies in computational structural biology and bioinformatics, especially for molecular dynamics (MD) simulations of biological macromolecules and their complexes.









MD Simulation Needs

- Resources to compute and store massive set of trajectories for further analyses
- End-users are biologists that don't have an experience with HPC and Grid computing









MolDynGrid Current Infrastructure

- Own production ARC CE (UA-IMBG) for computations and development
- Other most powerful CEs in Ukraine for production computing
- 80TB(own)+20TB grid-storage
 - MD trajectories database
 - Jobs data stage-in and stage-out
- MolDynSub CLI for jobs submission
- Web Portal for job submission and monitoring









MolDynGrid Web Portal

The first step towards the automation of MD computations in GROMACS for MolDynGrid objects back to 2009



- Submission via old ARC CLI
- Job status pulled from ARC Infosys
- Monitoring interface
- Trajectories Database with links to computation results Available at

https://moldyngrid.org

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MolDynSub CLI

Version <= 2.1

- Legacy ARC submission only
- GROMACS MD oriented
- Old portal backend



Version 3.x

- New modular design
- Different software modules
- Different infrastructures modules (Legacy ARC, ARC EMI-ES, Rainbow support)
- Different portal backends
 - new MolDynGrid portal backend with REST push notifications
 - old backend for backward compatibility





Different software needs for MD analyses

- Several versions of computational software
 - Including additional force-field builds
 - Additional analysis tools
 - Quantum chemistry modules
- All versions need to be compiled for each of the heterogeneous resources that run different operating systems



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Grid Solution for Wide Computing and Data Han

Rainbow ("ARC in the Cloud")

Running virtual machines as a grid jobs

□ to dynamically create interactive access platforms

□ to run software in pre-created environment







Rainbow JobWrap Mode

Transparent VM usage for computational jobs with minimal job description modifications

specify VM image location and request to invoke Rainbow JobWrap







BYOWN – Bring Your Own Worker Node

Docker Containers create own WN environment that runs under Rainbow
automated image maintaining framework
near zero overhead







EGI GPGPU FedCloud Resources



Page Discussion

MD simulations in GPU-accelerated NAMD

GPGPU-FedCloud

	EGI-Engage project:	IISAS: CloudLab		V/NA with ADC alignets	
Navigation		Project ^	Instances		VIVI WITH ARC Clients
Main page Community portal Current events Recent changes Random page Help		Compute ^			inside to fetch data
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	Applications being tested/running on HSAS-GF MolDynGrid http://moldyngrid.org/@ WeNMR https://www.wenmr.eu/@ Lifewatch-CC https://wiki.egi.eu/wil		FedC		

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Summary

- MolDynGrid Infrastructure rely on ARC components to compute jobs in both Grid and Cloud
- **Using flexibility of ARC** we have managed to
 - use existing grid infrastructure as a hardware provider for on-demand virtual machines with interactive access
 - automate software maintainability tasks in the heterogeneous grid environment
 - **stage data to the Cloud** from the grid storage network
- With those development on the top of ARC and ARC-powered grid infrastructure MolDynGrid solves valuable scientific problems*
- Methods and tools used are applicable to other research communities needs**

*Savytskyi OV, Yesylevskyy SO, Kornelyuk AI. Asymmetric structure and domain binding interfaces of human tyrosyltRNA synthetase studied by molecular dynamics simulations. J Mol Recognit. 2013;26(2):113–20. **If you are interested in running VMs in grid contact us: <u>grid@grid.org.ua</u>

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Thank you for kind attention!

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