ASTERIX

Adaptive Strategies Towards Expedient Recovery In eXascale

FAISER

Fast AI-based Space Environment Prediction

INNO4 SCALE

HELSINGIN YLIOPISTO

Research Council of Finland

Team

Participating here at Brussels:

- Kostis Papadakis [ASTERIX]
- Ioanna Bouri [FAISER]

- Juhani Kataja [ASTERIX] present at Brussels (but hacking away with the Elmer team).
- Markku Alho [ASTERIX] available remotely.

PIs:

- ASTERIX & Vlasiator & FAISER PI Minna Palmroth
- FAISER Co-I & CosCo PI Teemu Roos
- CSC ASTERIX Co-I Jussi Heikonen

Vlasiator

- 6D Global Hybrid Vlasov model that simulates the near-Earth space.
- 3D Velocity Distribution Functions (VDF) at every simulation cell.
- Massive resources for 6D simulations. Current runs are performed on 500 LUMI nodes.
- ~15-20 MCPUh or more for productions runs.
- Checkpoint mechanism for resilient restarting.
- Checkpoint files are 5-7 TiB for 3D production runs.
- Cannot have frequent restart files lying on disk.
- Fewer checkpoint files leads to wasted computational effort.

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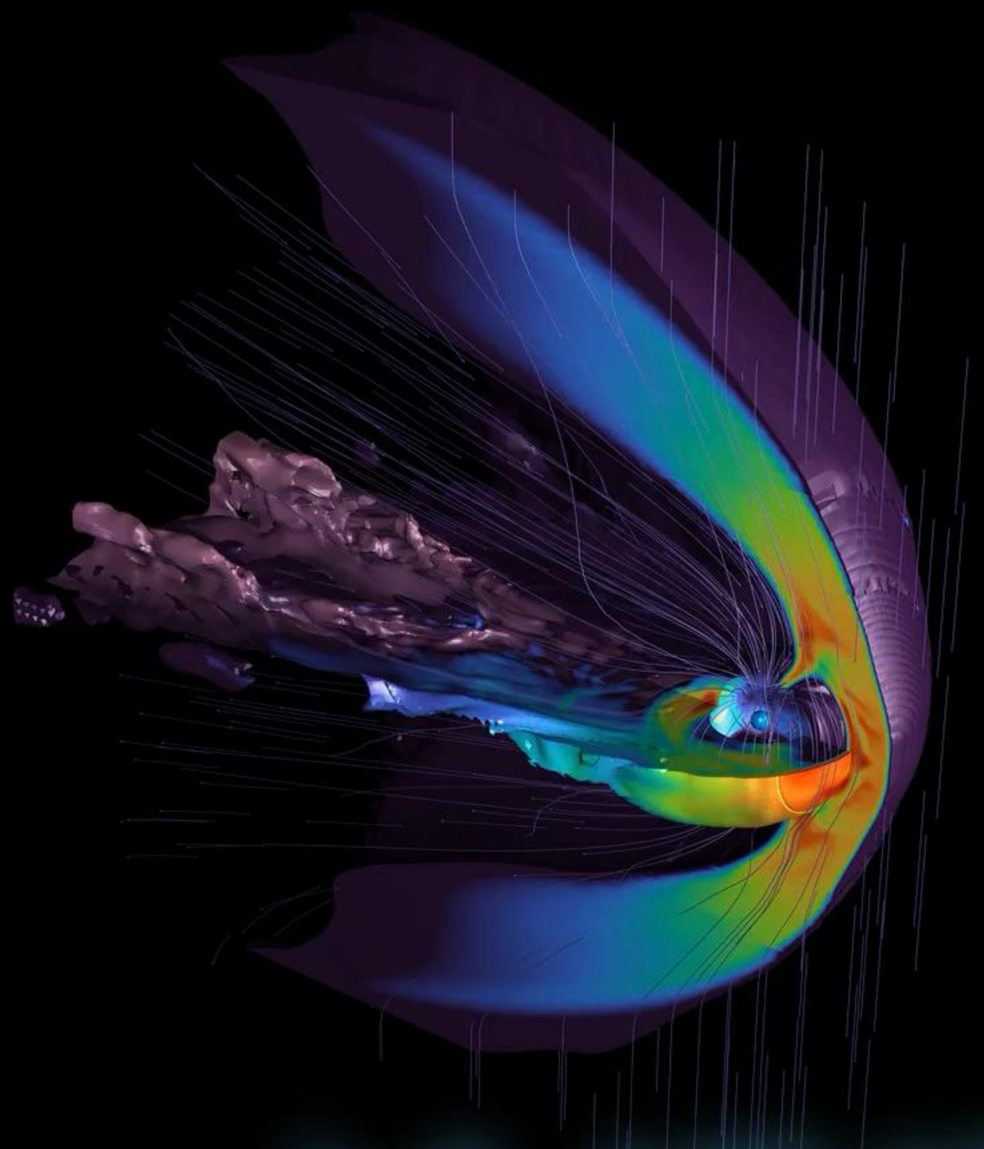

VLASIATOR

Vlasiator source code & details

- Vlasiator is written in modern C++.
- Parallelized over ~all available levels
  - MPI (domain decomposition, Zoltan)
  - OpenMP
  - Vectorization
- Currently our GPU branch with support for NVIDIA/AMD hardware is under development.
- Source code is hosted on GitHub at https://github.com/fmihpc/vlasiator.

- Solves the Vlasov equation of ion species:
  - 6D distribution (3D space, 3D velocity) propagated in time by shear transformations
  - Spatial AMR
  - Sparse representation of velocity space per spatial cell for memory efficiency (95% reduced memory footprint)

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Goals of Projects

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Compression of Vlasiator VDF data (with ML/AI methods, on GPUs) so that:

1) Compression is physically sensible (recovery from lossy restart)
2) Compression is fast enough (so that we can store lossy restarts often)

FAISER

1) 6D compressed/latent-space presentation of VDFs
2) Offloading Vlasov eq. propagation to happen solely in the latent space to obtain a fast solver
3) Bootstrap an AI "forecast model" with training data from fast simulations via 2)

Status

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Prototyping resulted in using Multilayer Perceptrons (MLPs) with Fourier features with Octree compression as a fallback; inconclusive results for vector-quantized variational autoencoder (VQ-VAE)

- MLP compression implemented in Vlasiator.
- GPU version of MLP under development.
- Octree method to be implemented.
- VQ-VAE inference model under development.

FAISER

Goals align with using autoencoders such as VQ-VAE, but see above

- RCF project online from 1st of September 2024
- Building on ASTERIX

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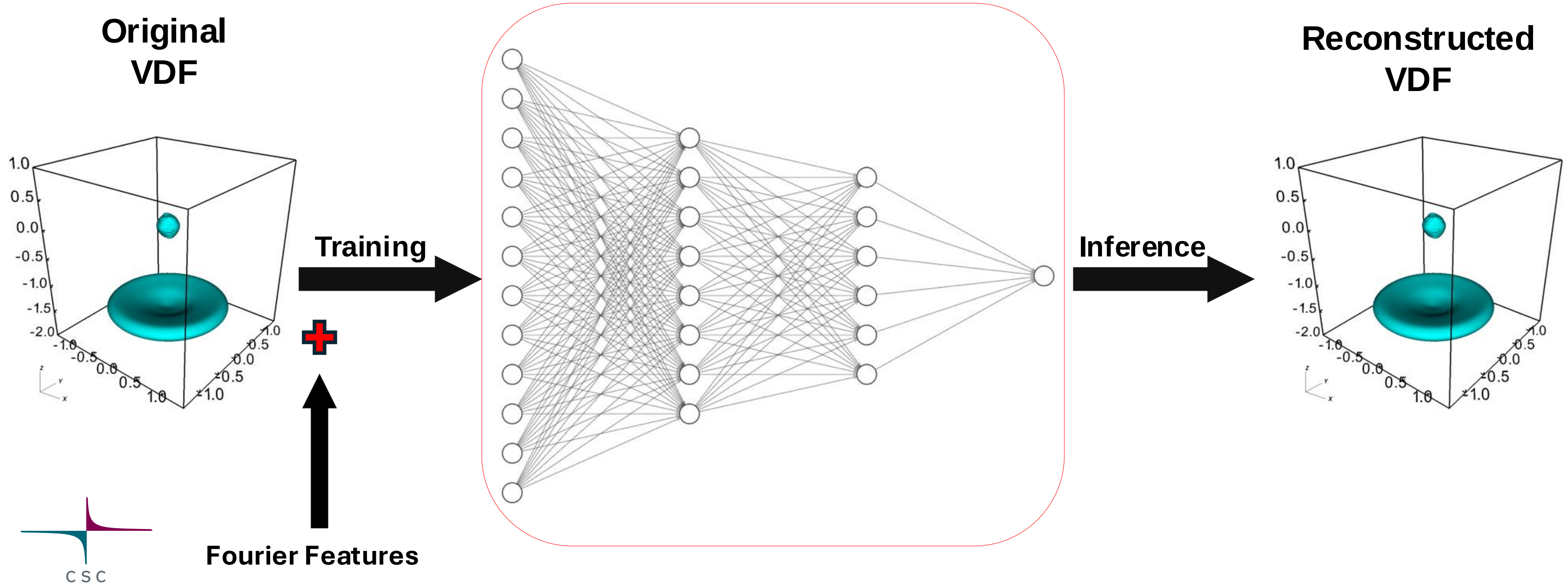
Using Neural Networks to compress VDFs [ASTERIX MLP]

- We are developing a Multilayer Perceptron to train on our VDFs during runtime.
- Fourier features encoding of input space.
- Network weights are stored instead of the original VDF voxel mesh.
- Network weights are updated at regular simulation intervals.
- MLP is trained on a subsampled version of the VDF to speed up training.
- VDF is recovered via inference.

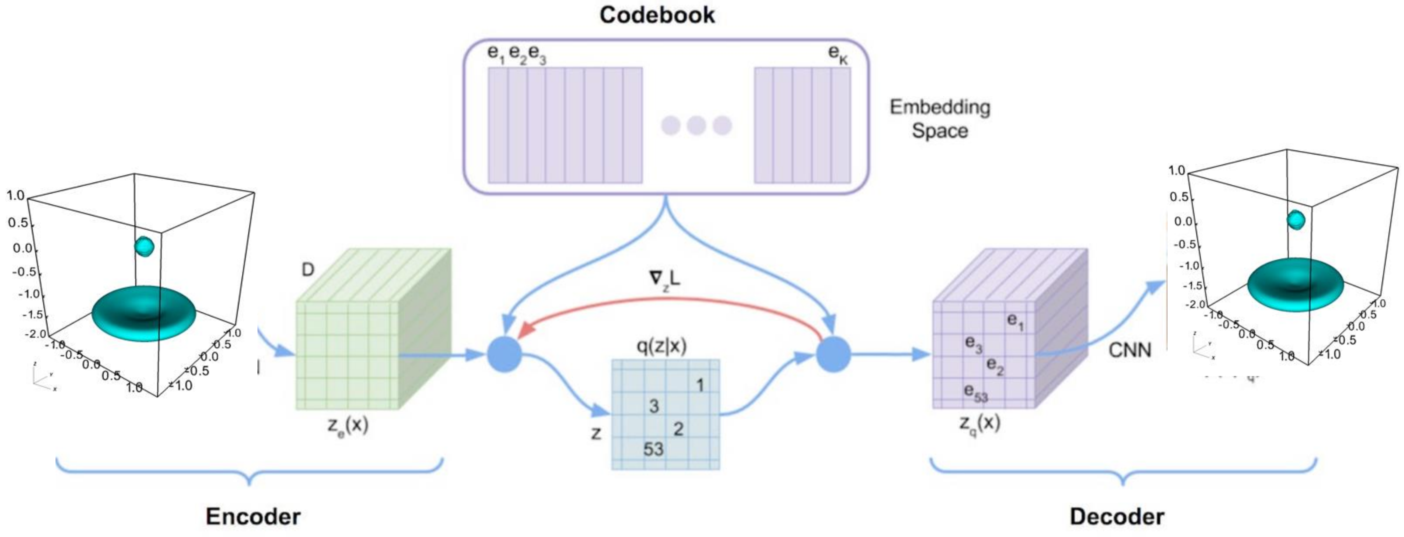


Using VQ-VAEs to compress VDFs [ASTERIX, FAISER]

- Objective: scaling a 3D VQ-VAE to train on existing restart files.
- Objective: extend the 3D VQ-VAE for time-dependent 6D data

- VQ-VAEs learn a discrete latent space representation of the input by incorporating a vector quantization (VQ) module at the bottleneck.
- Motivation: We developed a 3D VQ-VAE that can provide effective compressed state representations leveraging the sparsity of the input VDFs.

- The 3D VQ-VAE is a PyTorch DDP implementation.



Adapted from: Neural Discrete Representation Learning [van den Oord et al.]

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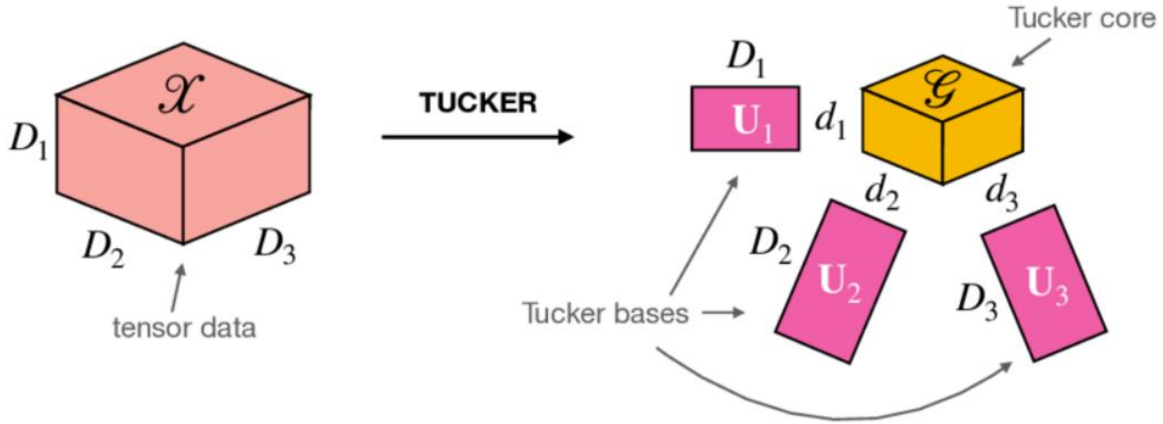
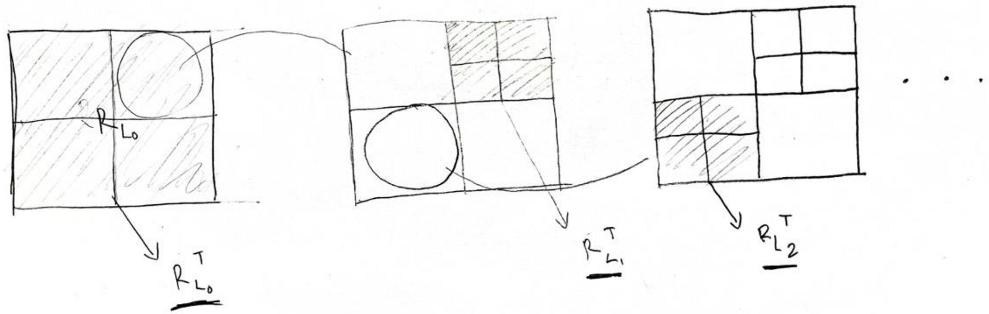
Multi-res Octree-Tucker Approximation of Gridded Data

... in case ML/AI methods don't work...

- Efficient compression and approximation of large 3D gridded data.
- Adaptive subdivision of the data into smaller cubical regions (leaf).
- Tensor factorization within cube with biggest residual using Tucker decomposition.
- Store factorizations and corresponding cube information.





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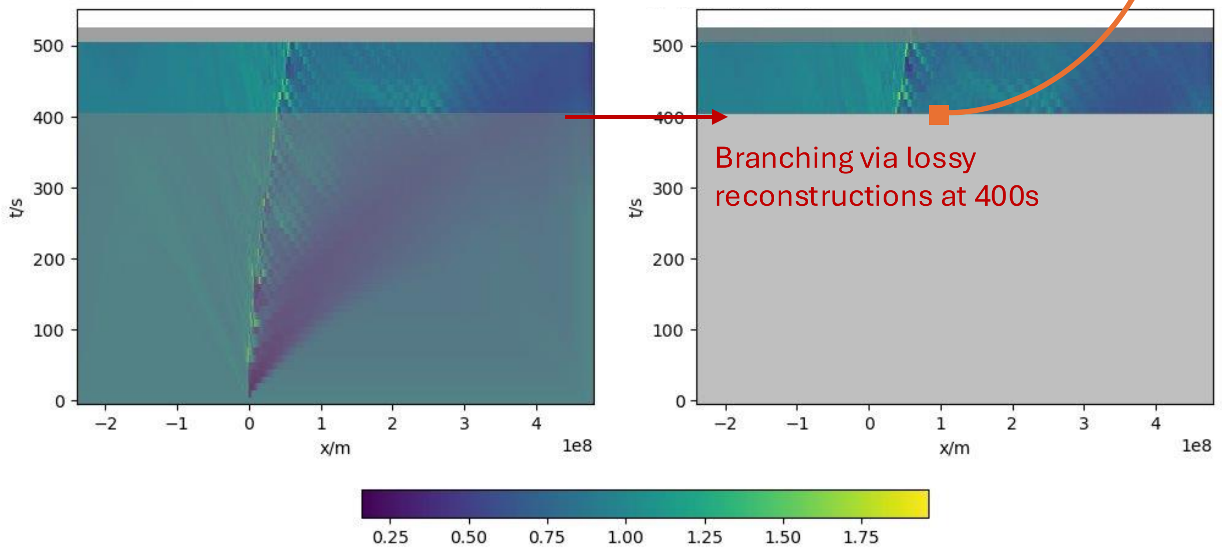
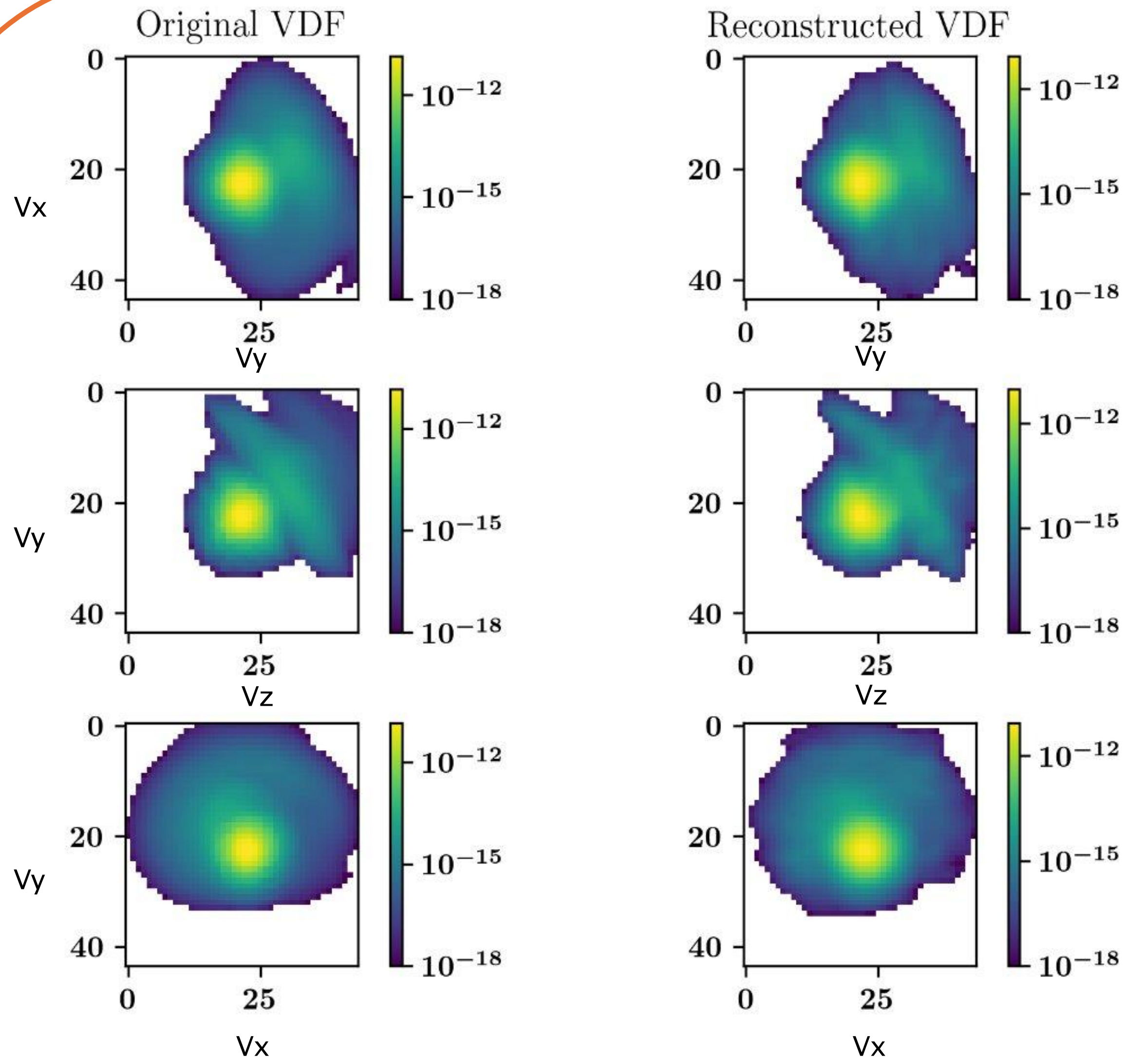
Restarting Vlasiator from a compressed state - proof of concept

1D shock tube simulation as a test case:
- develops nontrivial VDFs
- Dynamics dependent on reconstruction quality

Evolution of temperature anisotropy in a shock test run.



Single VDF from the shock run compressed 83 times



Hackathon goals

- Task 1: Scaling, tuning and training the 3D VQ-VAE prototype (ASTERIX)
- Task 2: Vlasiator restart data compression to GPUs (ASTERIX)
- Task 3: Scaling, tuning and training of the 6D VQ-VAE with temporal propagation (FAISER)
- Task 4: Vlasiator runtime hooks / online training of 6D VQ-VAE (FAISER)

Task 1) 3D VQ-VAE training at scale

- Problematic scaling so far. Implemented on PyTorch DDP.
- Not able to run on more than 10 LUMI-G nodes. Situation post LUMI-update?

- Goal: Training run on Vlasiator restart file(s), á 5 TiB

- Current implementation:
- Custom dataloader w/ cached disk reads
- https://github.com/kstppd/asterix/tree/vdf_replace/src/assessment/vqvae
- PyTorch support on AMD hardware & over MPI?
- Dataloader optimizations? Dep. on analysator for reading in data

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Task 2) Enable GPU training for MLP

- Use GPU partition to train the MLP during Vlasiator runtime.
- Use stream events to synchronize training.
- Evaluate performance against CPU training, test scaling.

Currently:

- Prototype running on CUDA, HIP-supported.
- Written in modern C++.
- Custom implementation using a Matrix class that supports CUblas/HIPblas operations.

Task 3) 6D VQ-VAE

- Toy-model dataset to be produced for hackathon
- Prototype autoencoder to be produced for hackathon

- Task: Expand Task 1 to enable training on the 6D dataset and with 6D autoencoders – at least at “small scale” without online training
- Will require more involved dataloaders, optimization, tuning...

Task 4) Runtime hooks in Vlasiator

- Interface to expose VDF data from Vlasiator runtime to training process. Below are the current ideas for approaching the topic

- Potentially implement a client server interface in Vlasiator.
- Split communicator probably using MPDP.
- Use MPI's dynamic process management.
- Create a synchronization scheme between communicators.
- Query VDFs and send them to parent communicator for online training?

- To be worked/discussed on as time allows during the hackathon.

Restarting Vlasiator from a compressed state extra example

Growth Rate of a 2D Kelvin Helmholtz Instability in Vlasiator.