EXASCALE MHD SIMULATIONS WITH

Cholla

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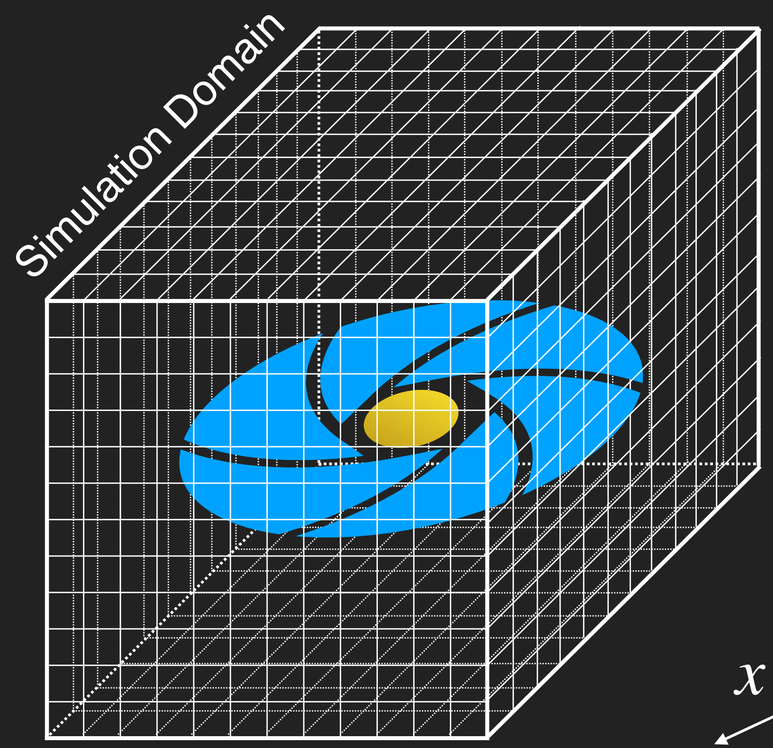
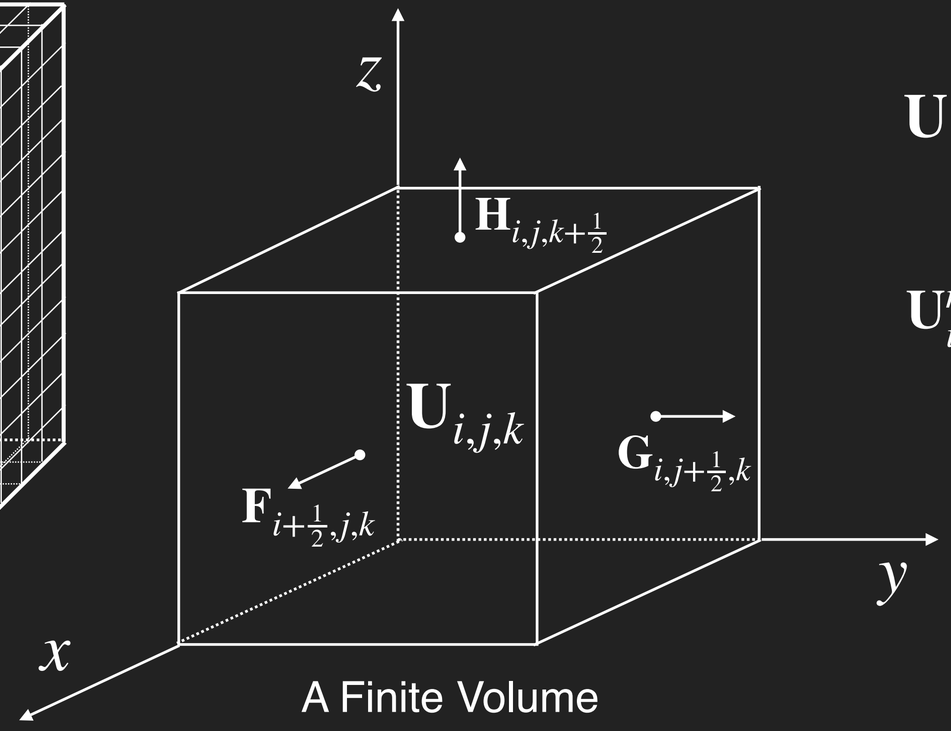
JSI WORKSHOP OCT. 11, 2023

Cholla is a GPU-native, massively-parallel, **finite-volume** hydrodynamics code developed for astrophysics simulations.



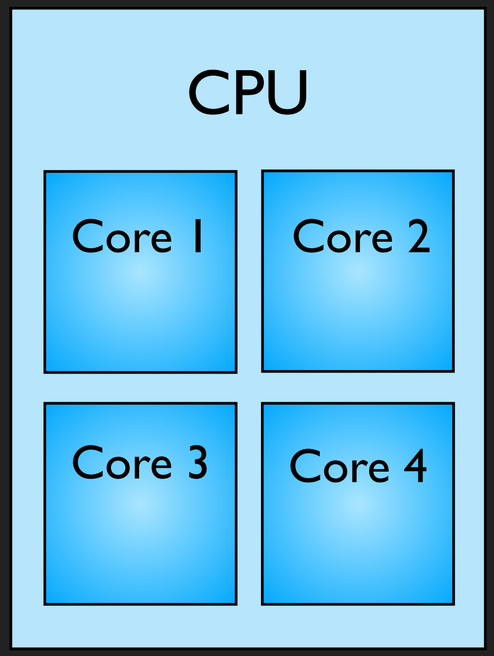


A Finite Volume

$$\mathbf{U} = [\rho, \rho u, \rho v, \rho w, E]^{\mathrm{T}}$$

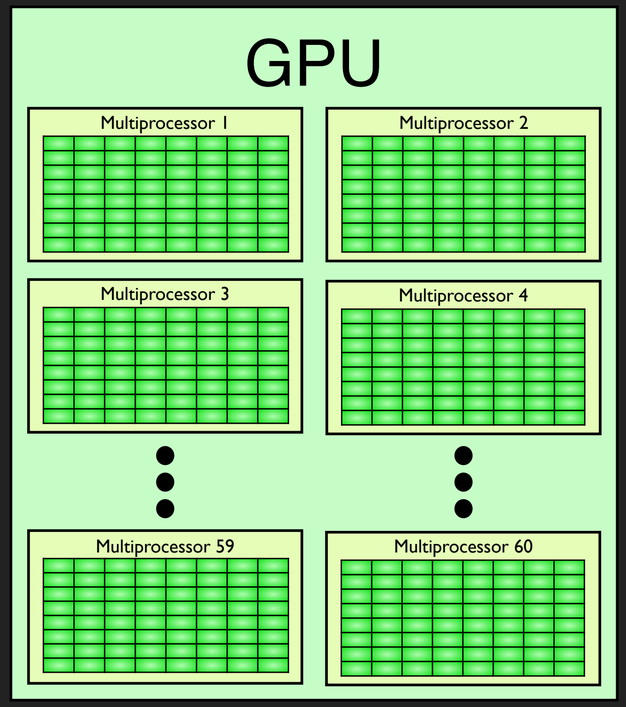
$$\mathbf{U}^{n+1}_{i,j,k} = \mathbf{U}^{n}_{i,j,k} - \frac{\delta t}{\delta x}\left(\mathbf{F}_{i+\frac{1}{2},j,k} - \mathbf{F}_{i-\frac{1}{2},j,k}\right) - \frac{\delta t}{\delta y}\left(\mathbf{G}_{i,j+\frac{1}{2},k} - \mathbf{G}_{i,j-\frac{1}{2},k}\right) - \frac{\delta t}{\delta z}\left(\mathbf{H}_{i,j,k+\frac{1}{2}} - \mathbf{H}_{i,j,k-\frac{1}{2}}\right)$$

WHY GPUs?



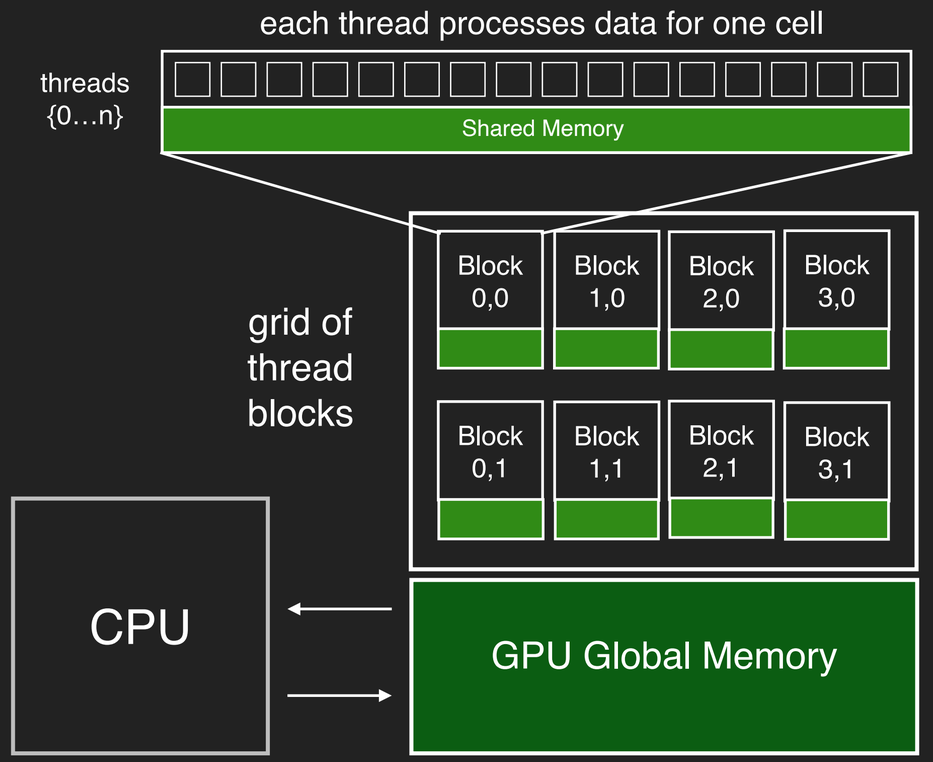
Optimized for Serial Tasks

~1-2 TFLOPS
≤128 cores
~4 GFLOPS/Watt

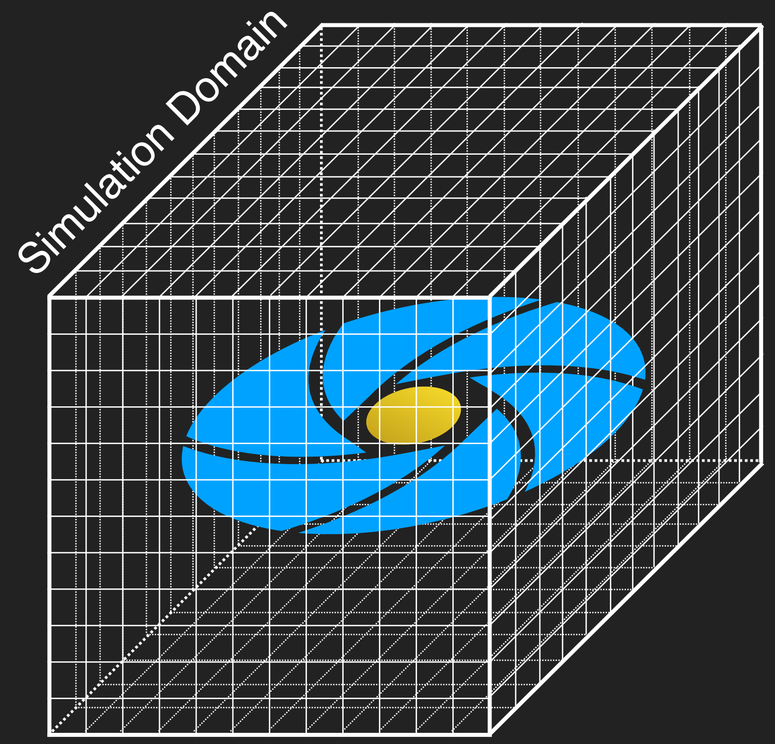


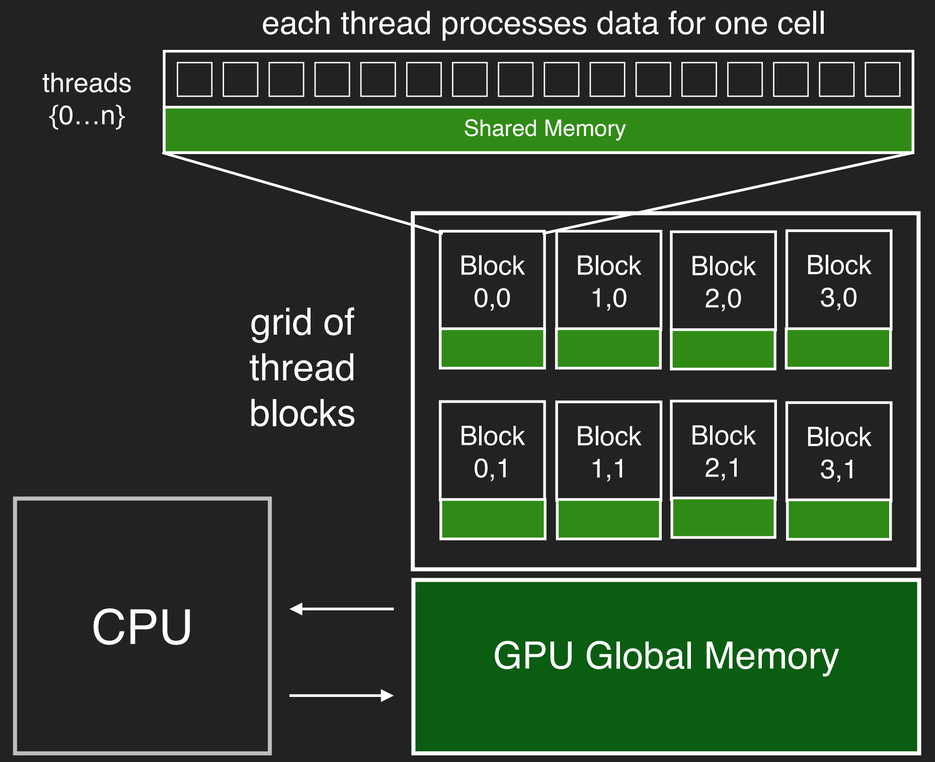
Optimized for Parallel Tasks

~30 TFLOPS
>7,500 cores
~50 GFLOPS/Watt



WHY GPUs?


Simulation Domain


each thread processes data for one cell
threads
{0…n}
Shared Memory
grid of
thread
blocks
Block
0,0
Block
1,0
Block
2,0
Block
3,0
Block
0,1
Block
1,1
Block
2,1
Block
3,1
CPU
GPU Global Memory

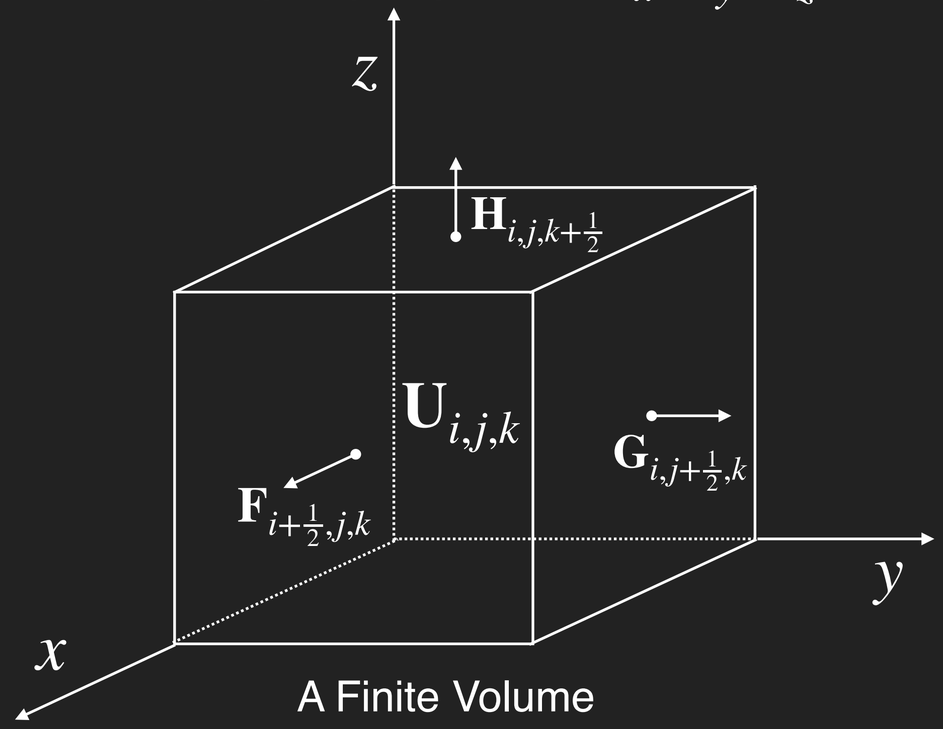
WHY CHOLLA MHD?

- No consensus on the effect of magnetic fields in galaxies
- Zero divergence methods are computationally expensive
  - $\nabla \cdot \overrightarrow{B} = 0$, magnetic monopoles shouldn't exist
- Need ~1pc resolution, impossible before the exascale era
- Required for anisotropic diffusion & cosmic ray transport
- Simulation data will be extensive and public

HOW TO REPRESENT THE MAGNETIC FIELD?

- Option 1:
  - Problems:
    - Transform the Induction equation
    - Non-zero divergence
  - Solution:
    - “Divergence Cleaning”, more computation and potentially insufficient

$$\mathbf{U} = [\rho, \rho u, \rho v, \rho w, E, B_x, B_y, B_z]^{\mathrm{T}}$$

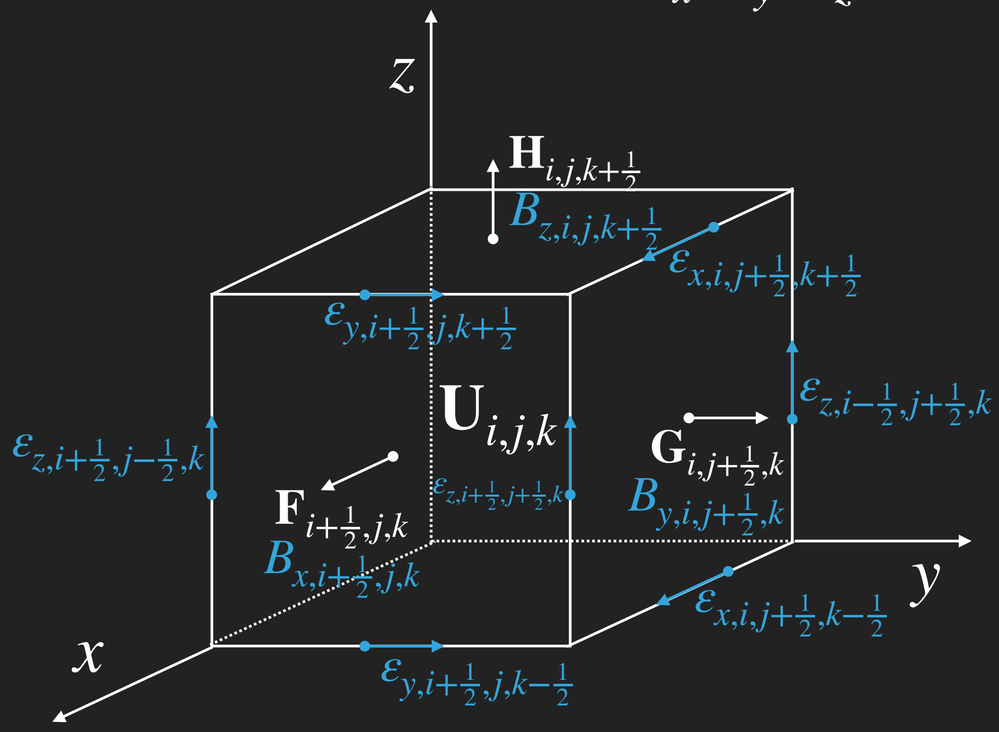


A Finite Volume

HOW TO REPRESENT THE MAGNETIC FIELD?

- Option 2: Constrained Transport
  - Divergence Free by construction
  - Computationally expensive
  - Complex to implement
  - Requires divergence free initial conditions

$$\mathbf{U} = [\rho, \rho u, \rho v, \rho w, E, B_x, B_y, B_z]^{\mathrm{T}}$$



A Finite Volume + Constrained Transport

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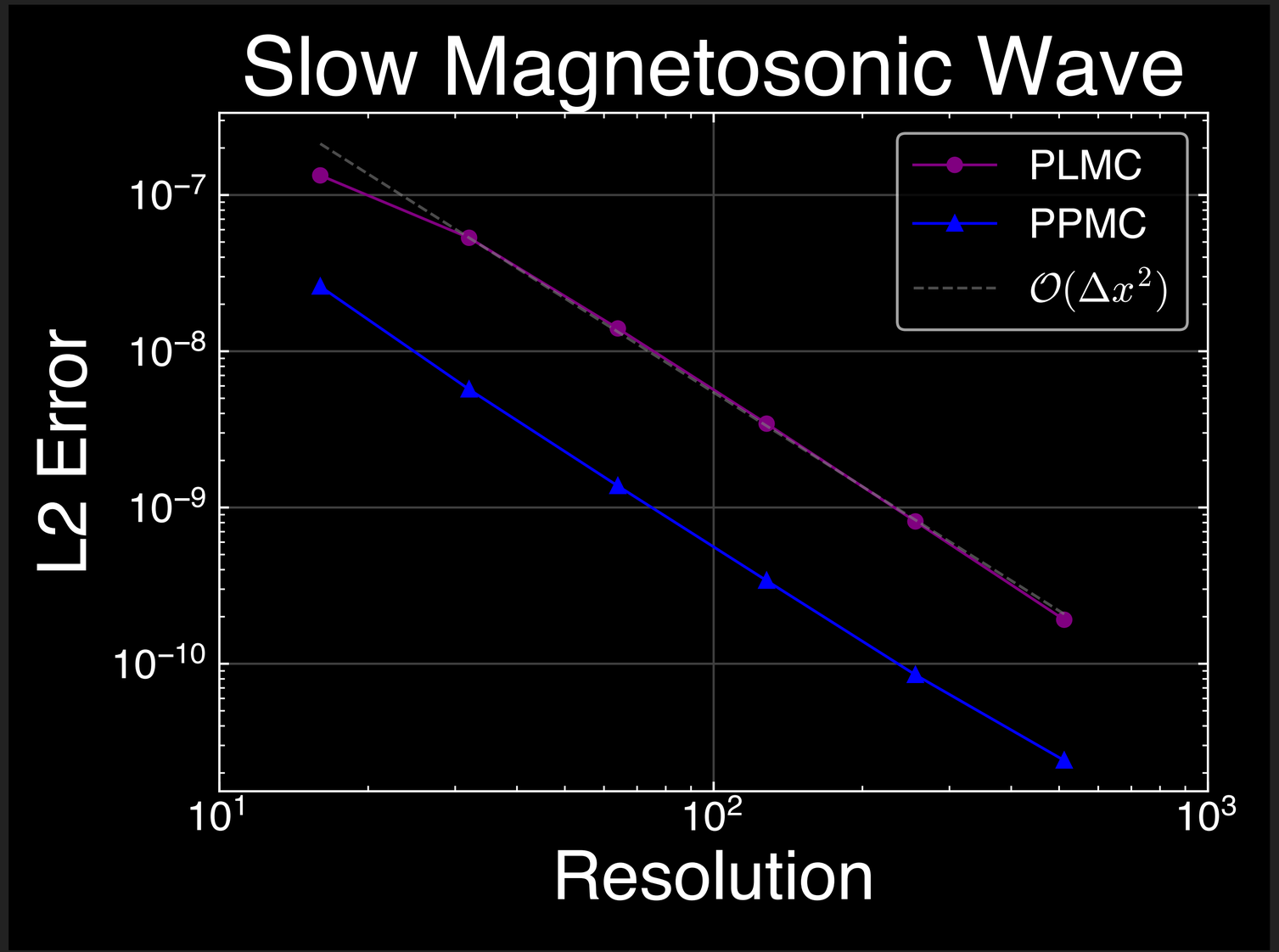
LINEAR WAVE CONVERGENCE



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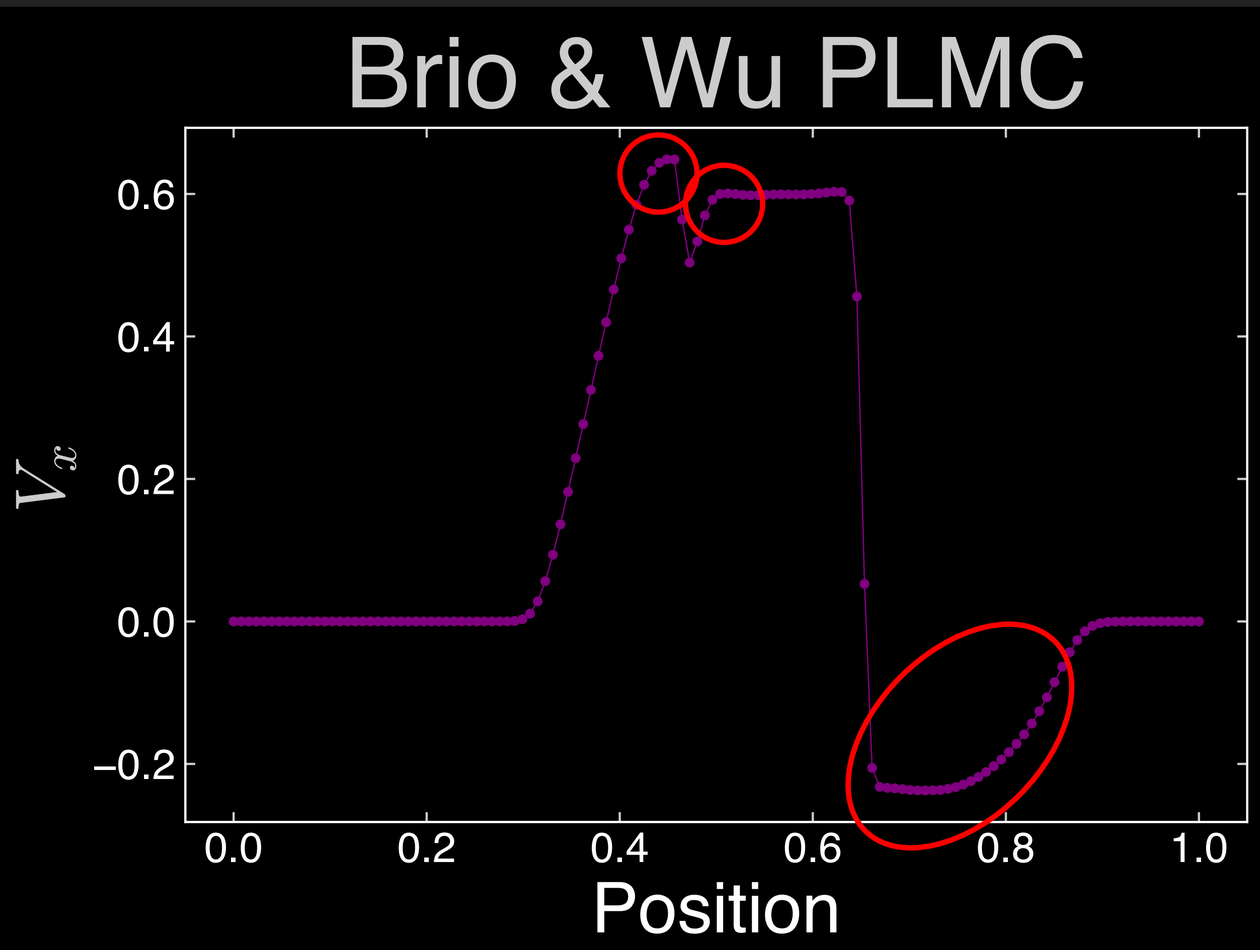
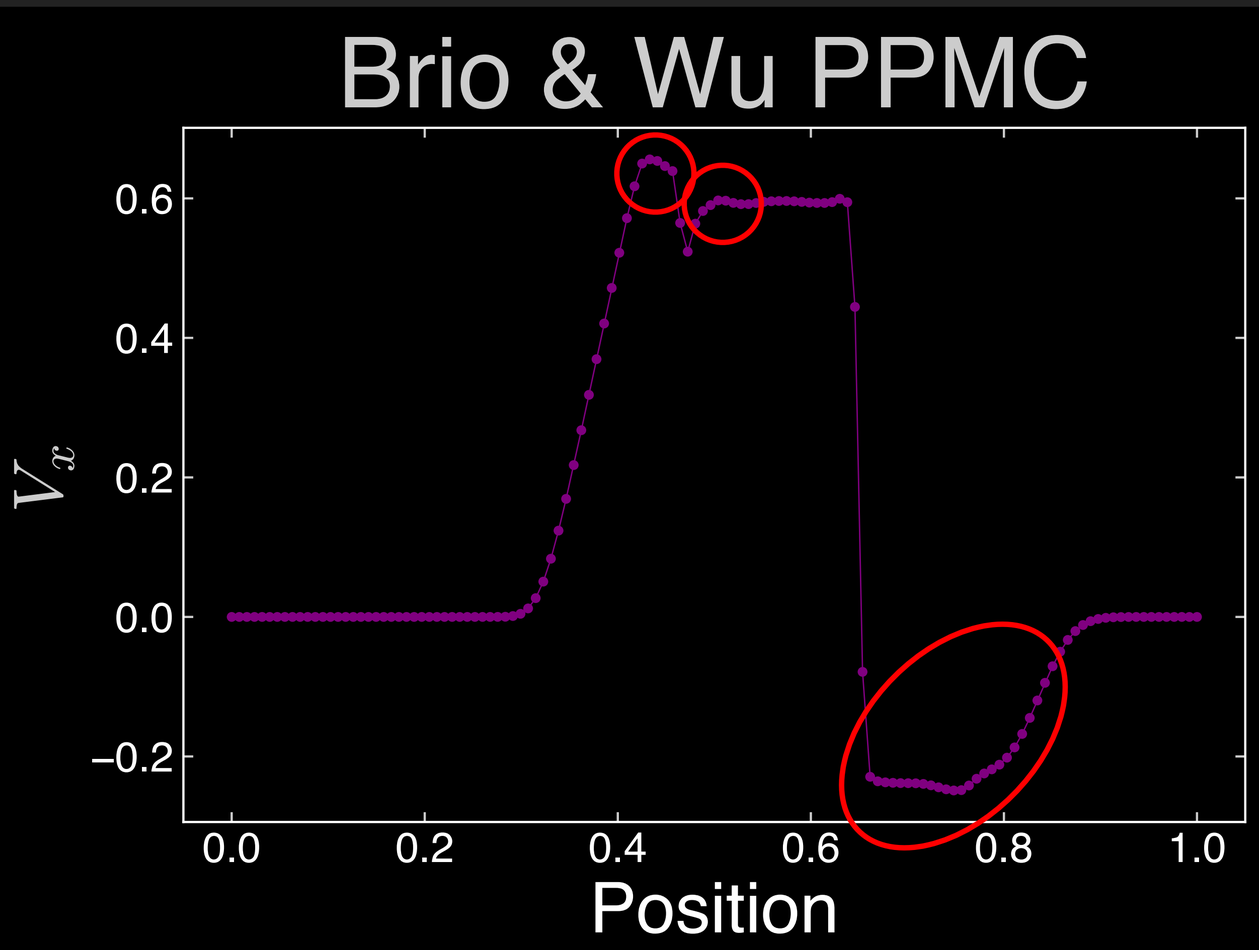
PPMC VS. PLMC – SHOCKS





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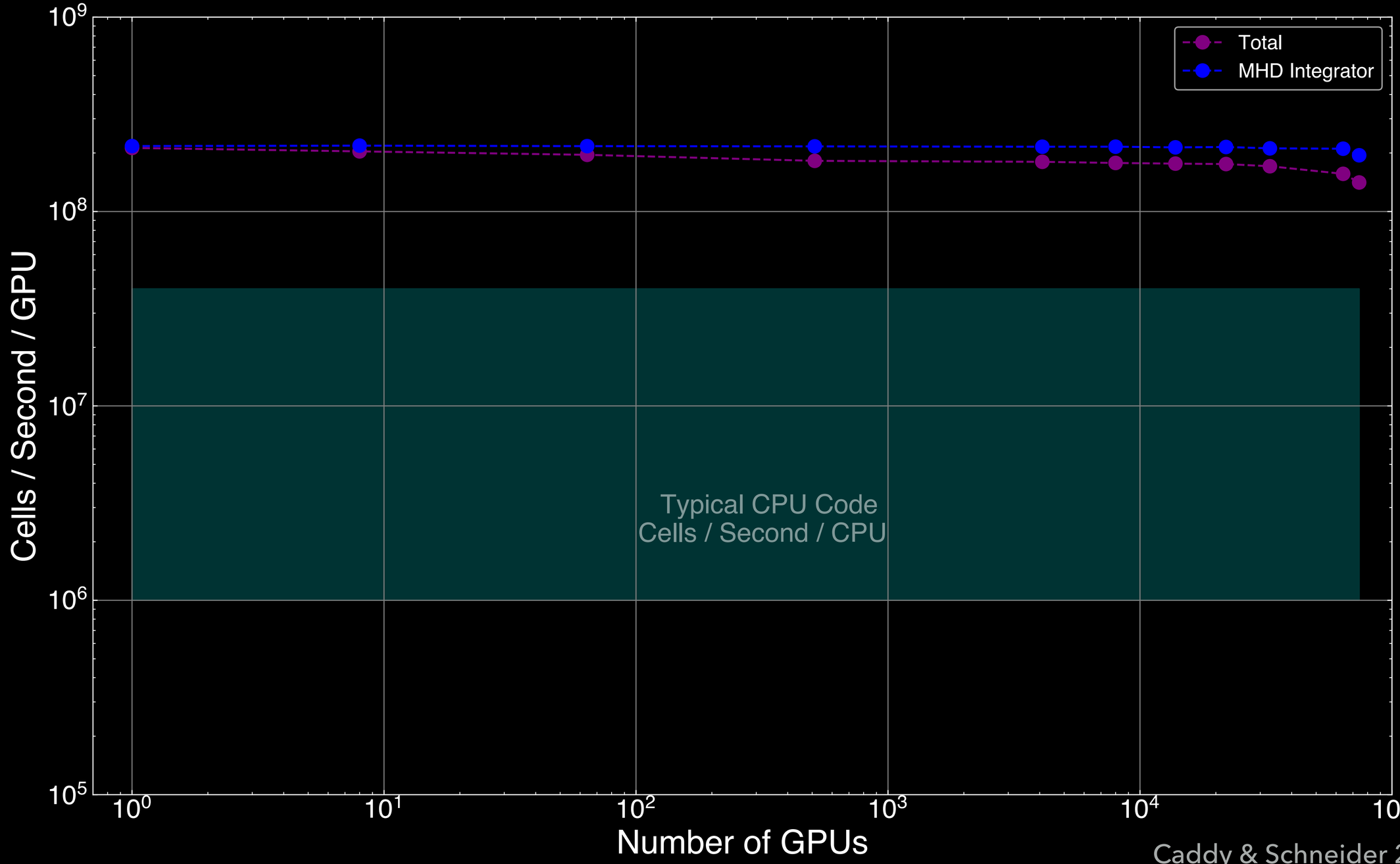
MHD Weak Scaling on Frontier (PLMC)



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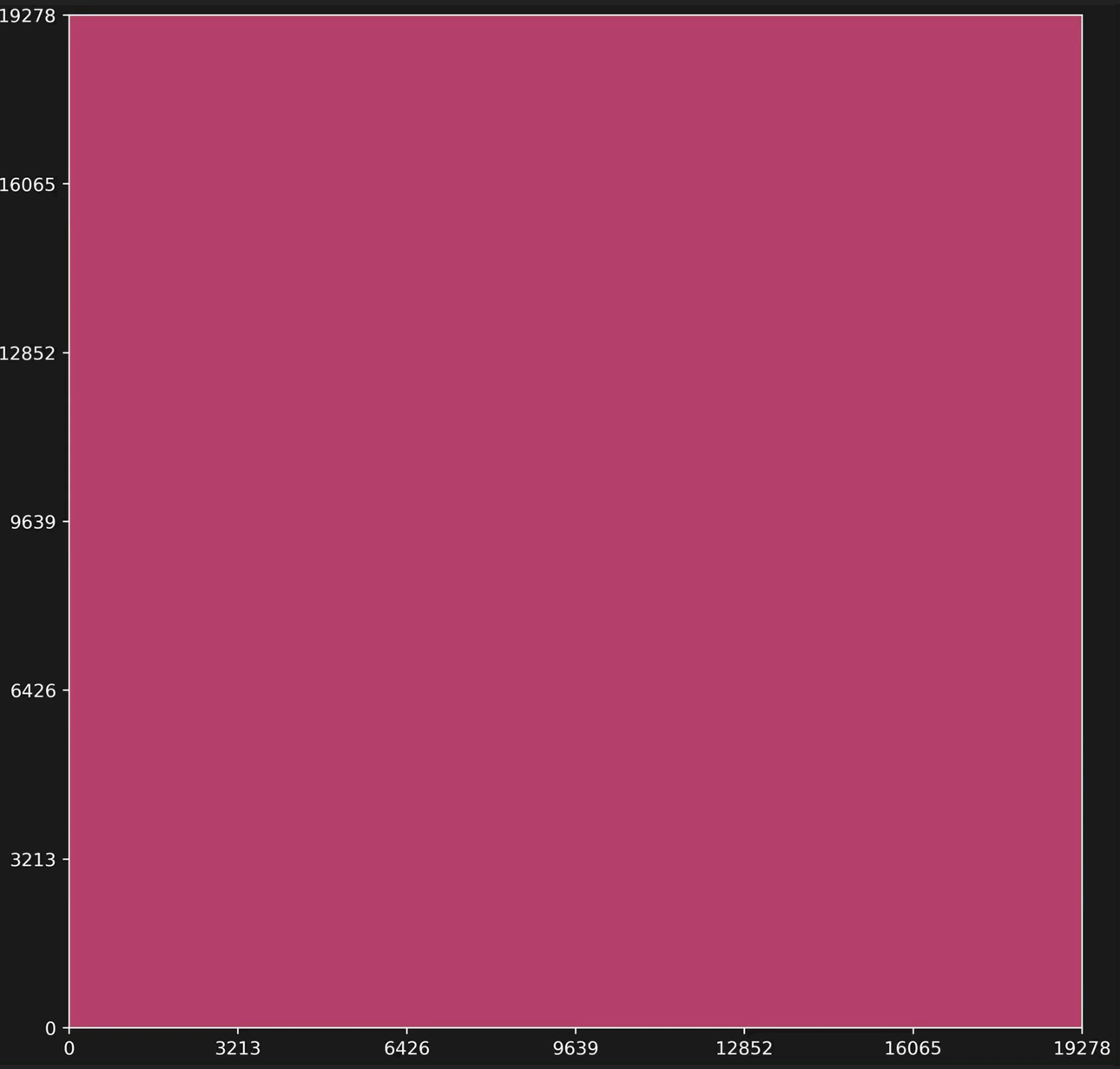
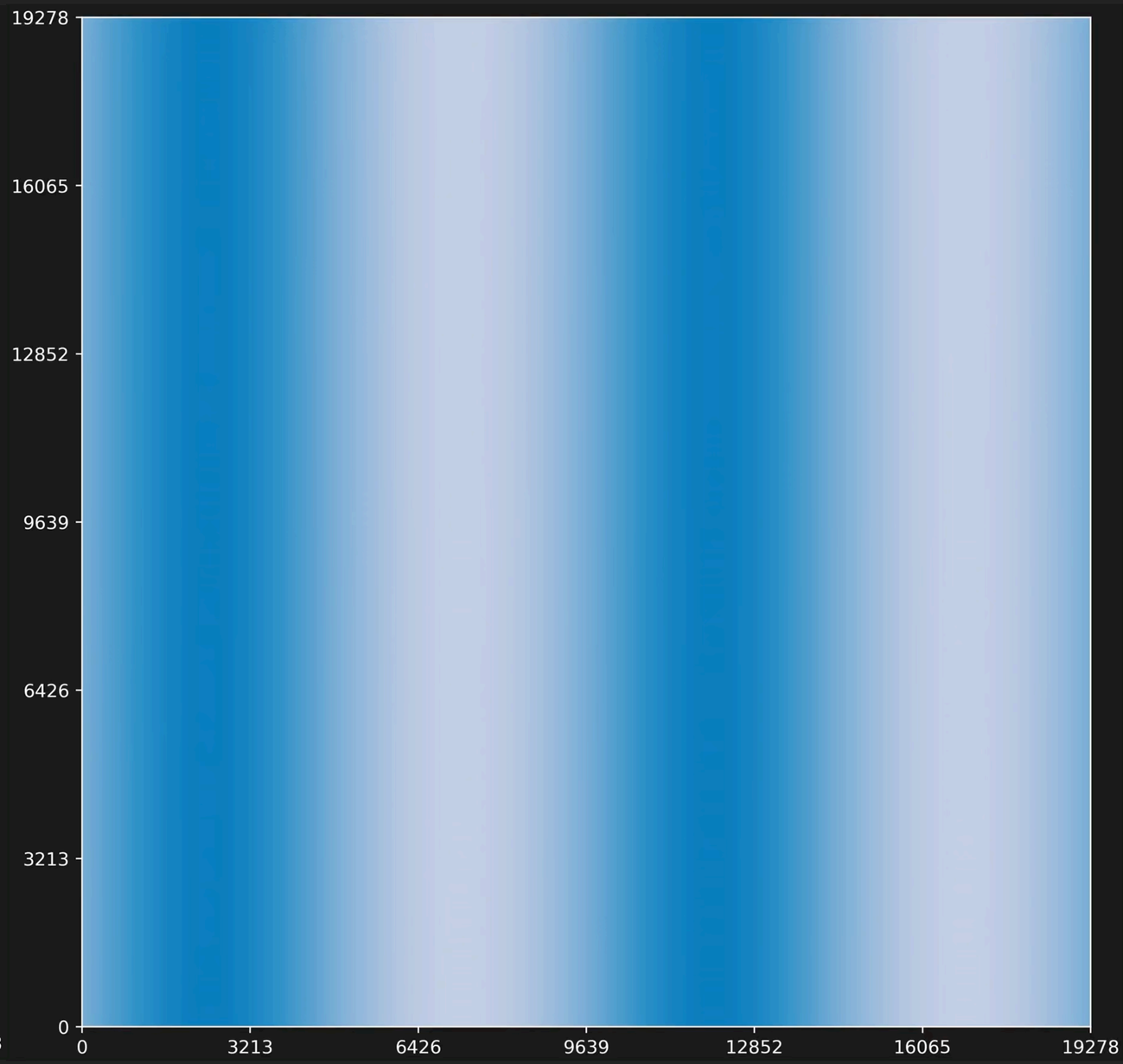
DENSITY

ORSZAG-TANG VORTEX

B_x





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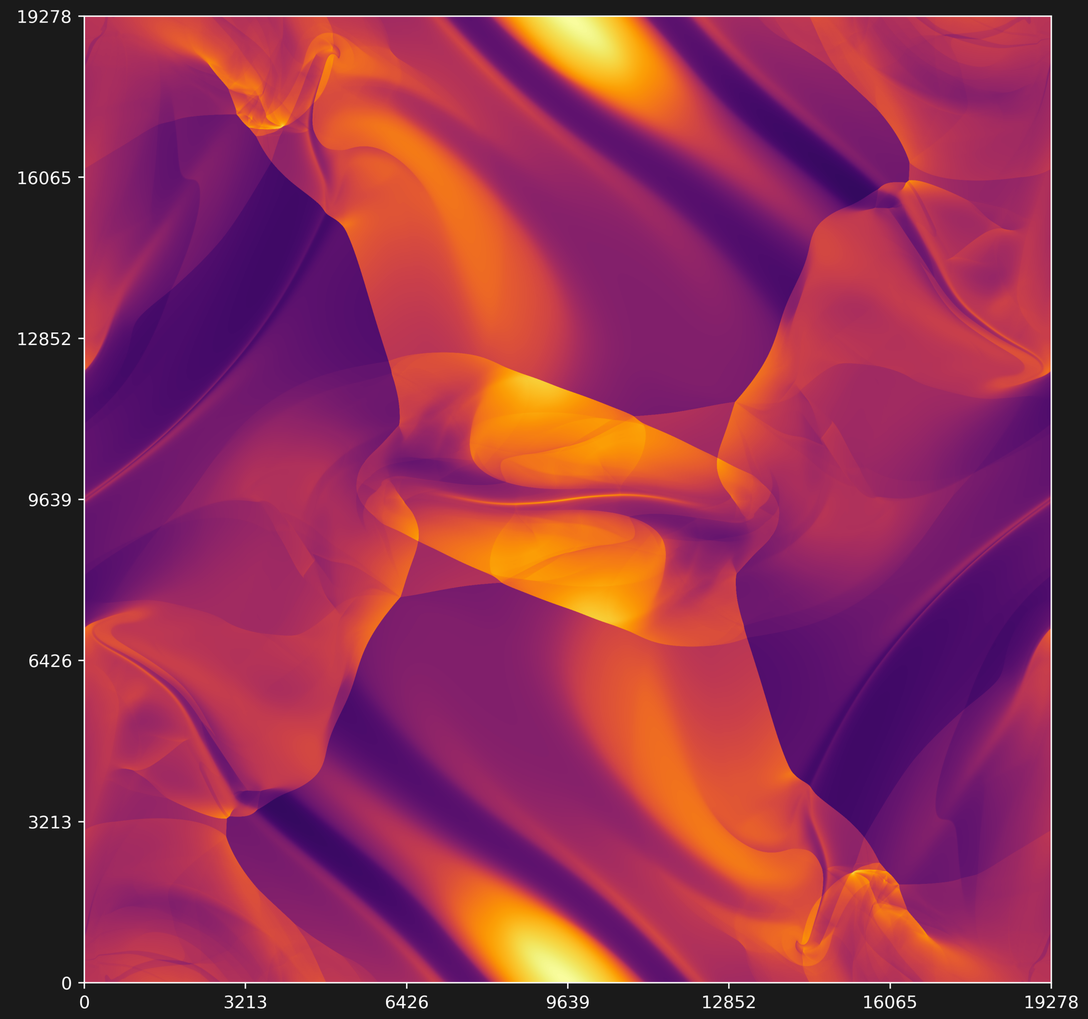
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9639
6426
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0
0
3213
6426
9639
12852
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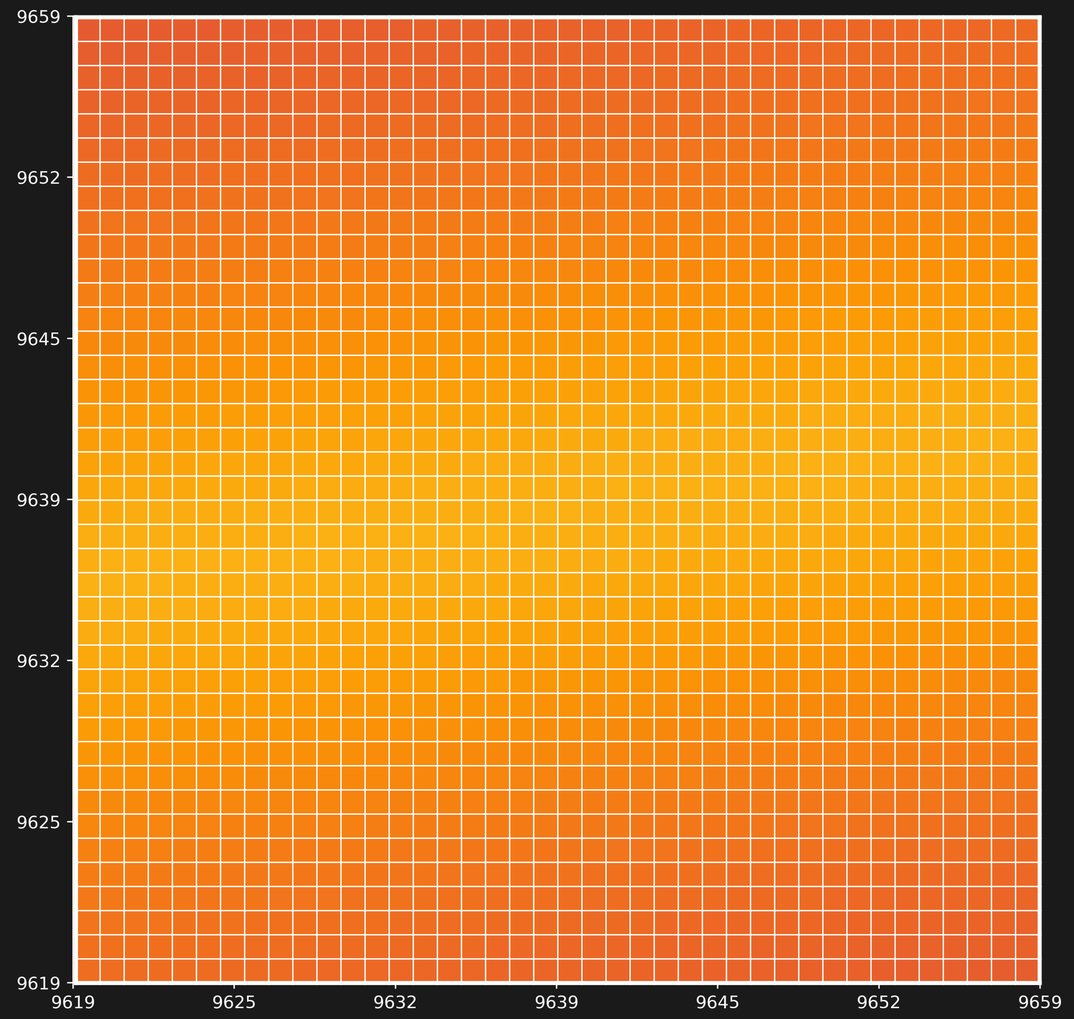
19278


9659
9652
9645
9639
9632
9625
9619
9619
9625
9632
9639
9645
9652
9659

TESTING & CONTINUOUS INTEGRATION (CI)

- Added a testing framework
- Tests are easy & fast to run with a single shell command
- Easy to add and change code confidently
- Tests are automated and run with each Pull Request (PR)
- Code formatting & static analysis (clang-tidy) also run on each PR

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CONCLUSION

- Cholla MHD is an exascale capable astrophysical MHD code
- The MHD module uses constrained transport to maintain zero divergence
- Includes a testing framework & automated testing/CI of all PRs
- Details in Caddy & Schneider 2023 in prep
- Cholla: github.com/cholla-hydro/cholla
- Resume, CV, etc: robertcaddy.com
- Talk Repo: github.com/bcaddy/JSI_Workshop_Talk_2023

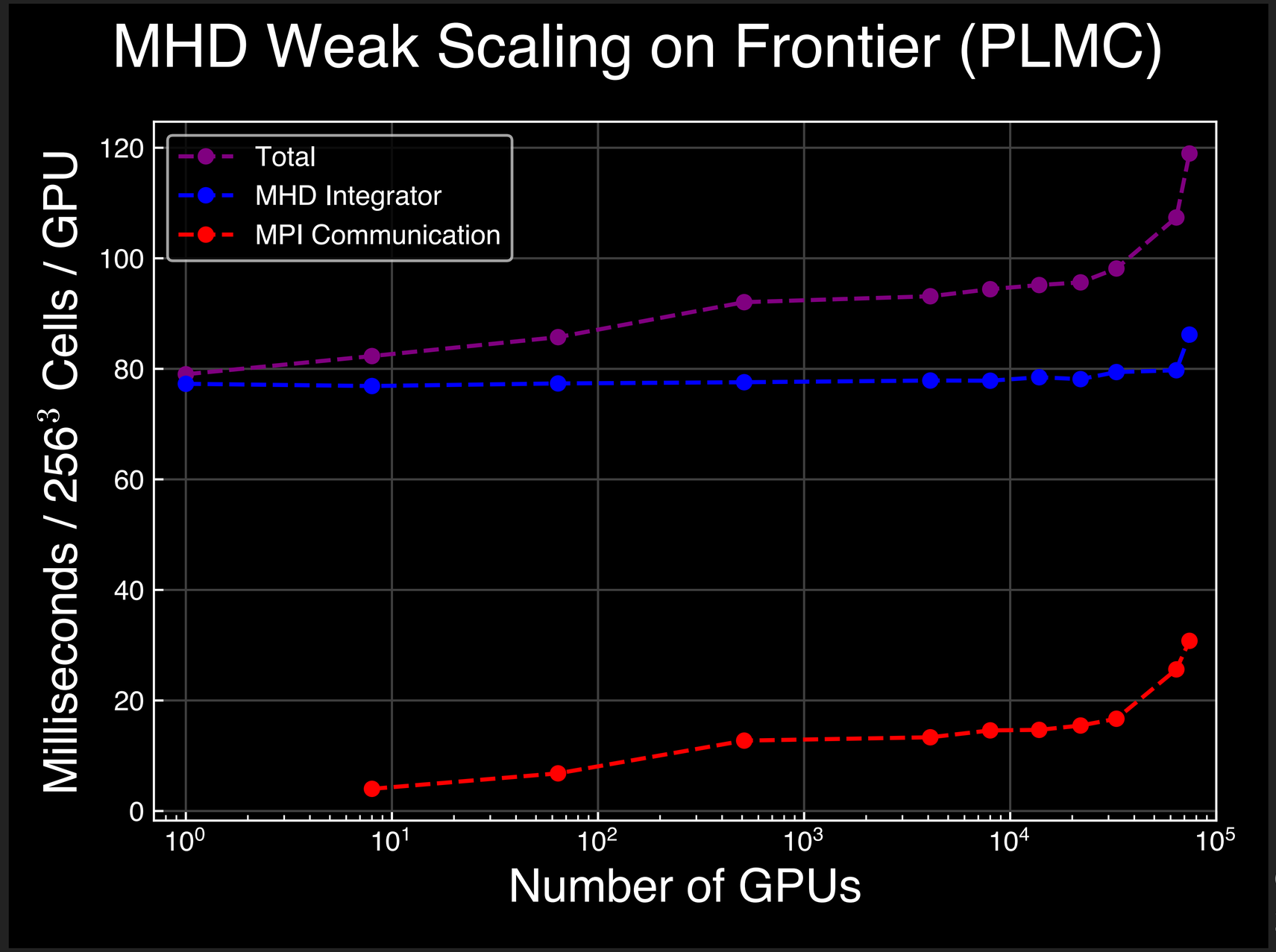
ADDITIONAL SLIDES

robertcaddy.com

github.com/bcaddy/JSI_Workshop_Talk_2023

github.com/cholla-hydro/cholla

SCALING PLOTS



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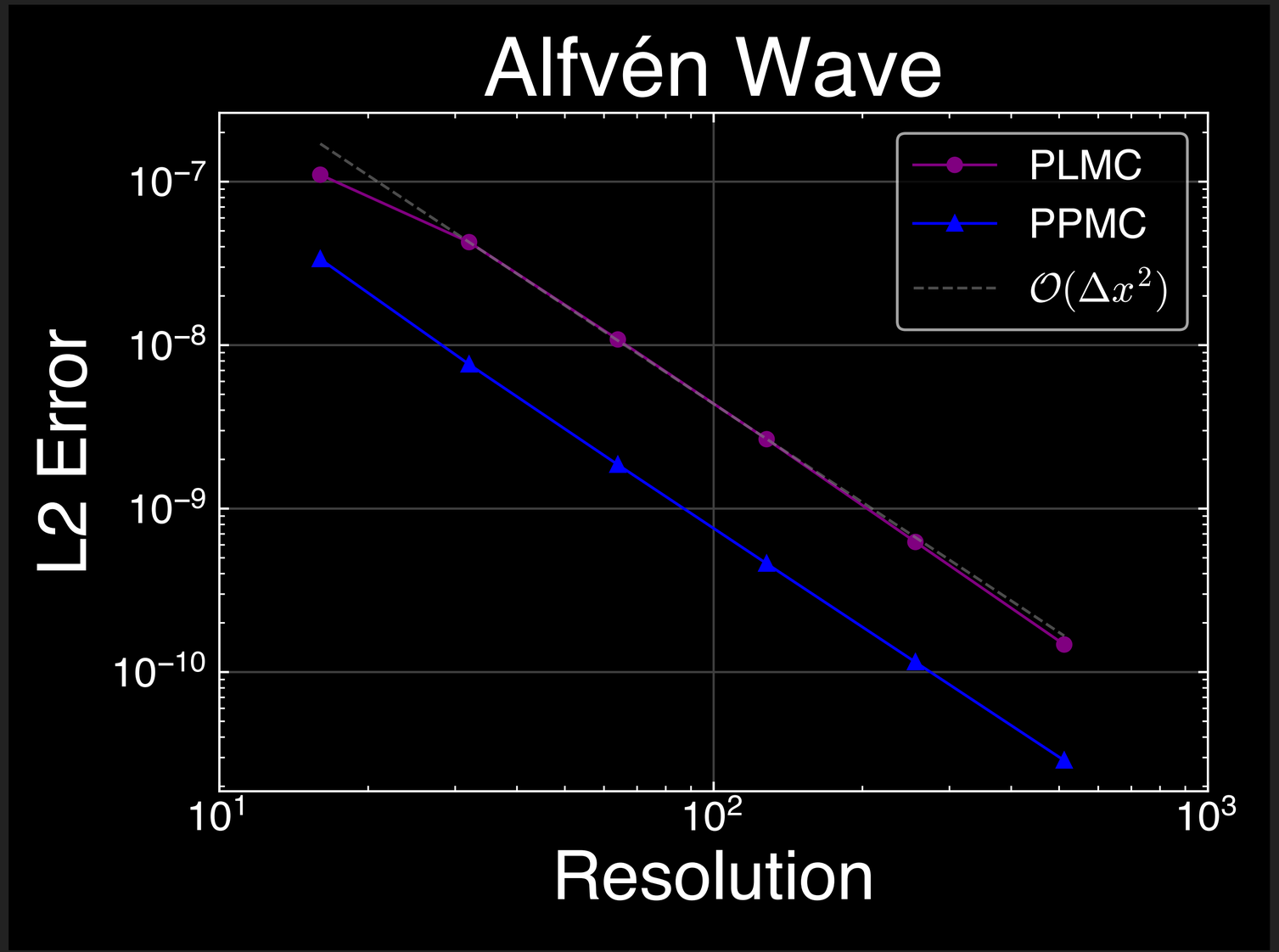
LINEAR WAVE CONVERGENCE



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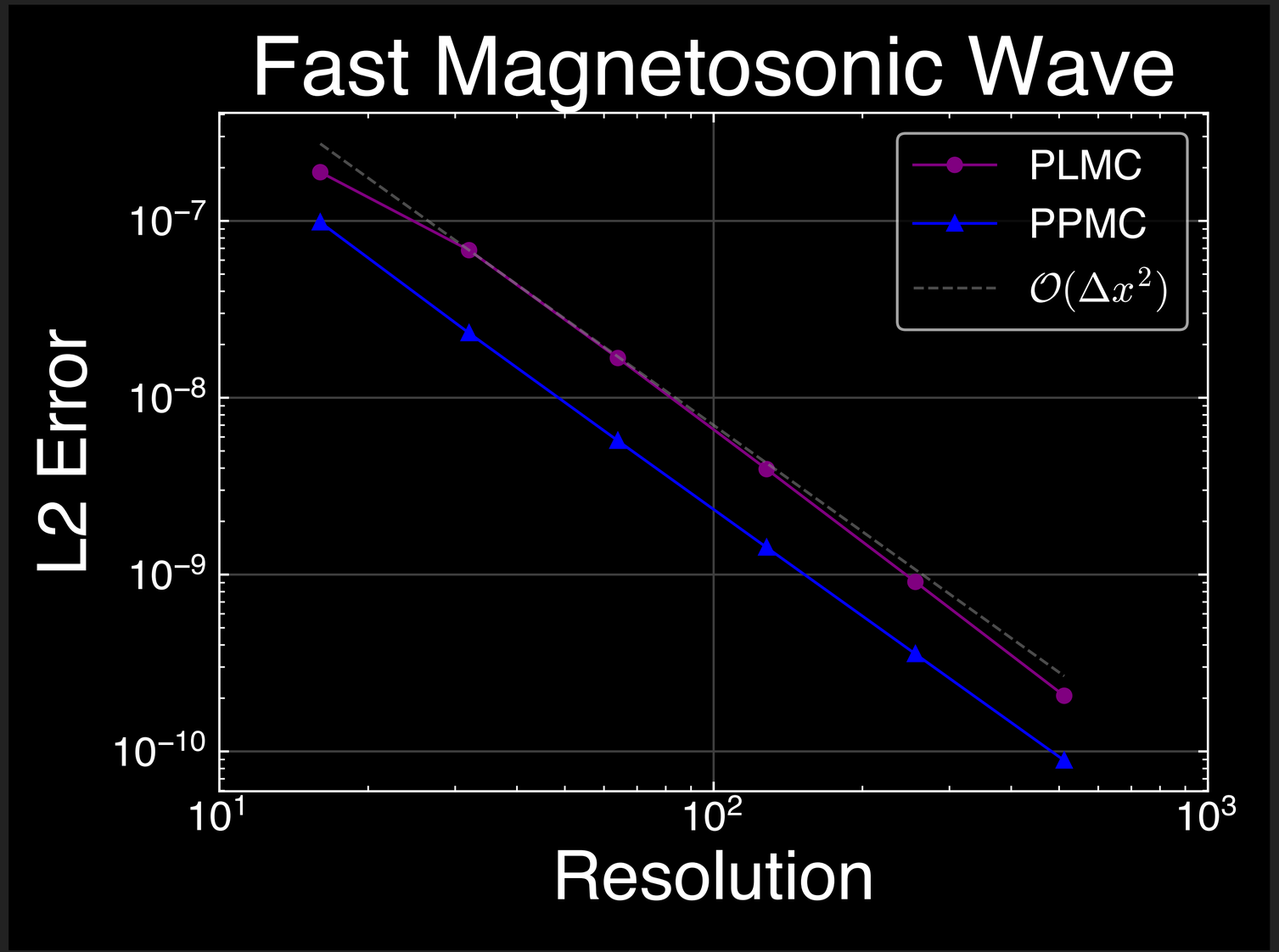
LINEAR WAVE CONVERGENCE



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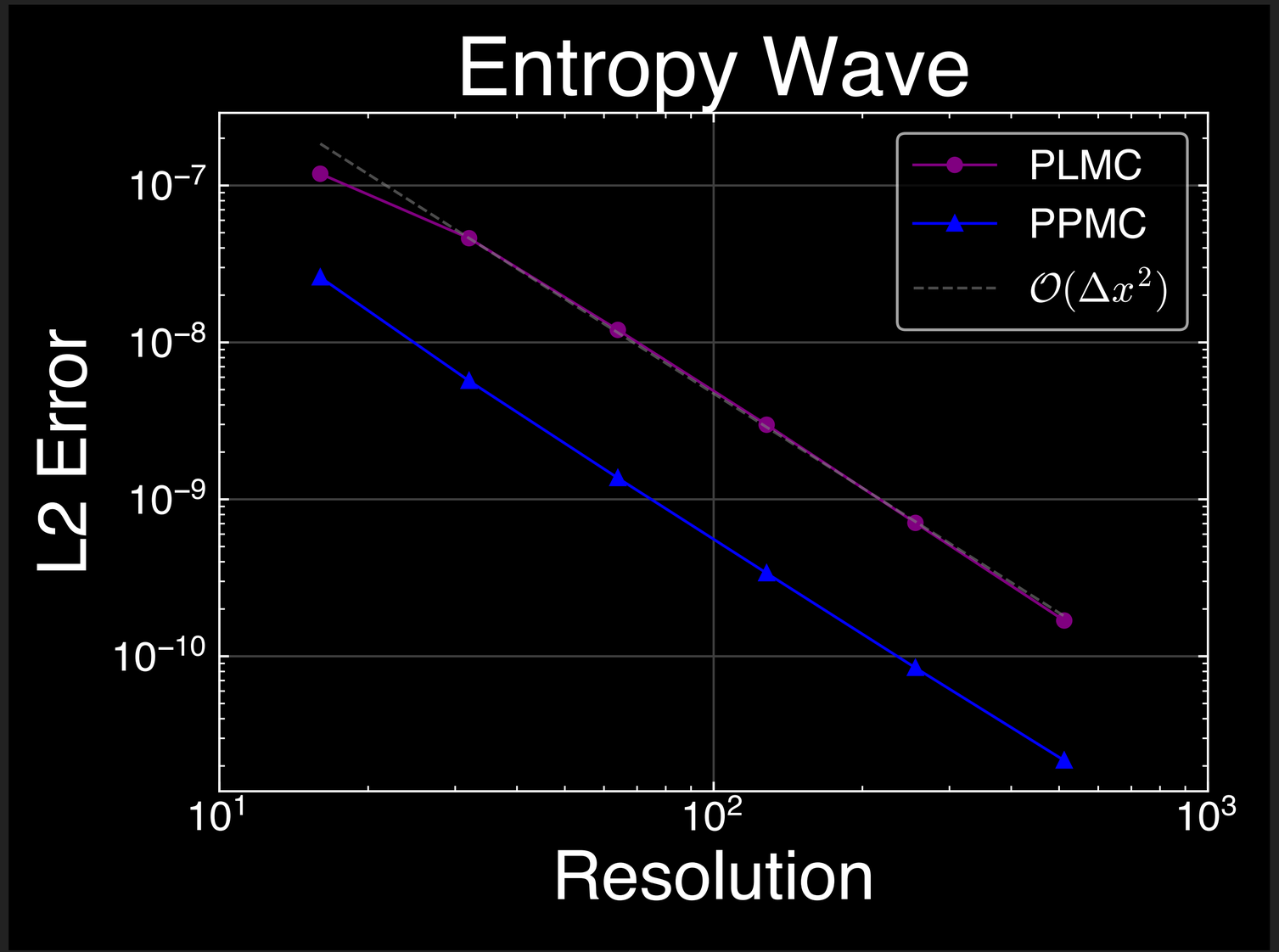

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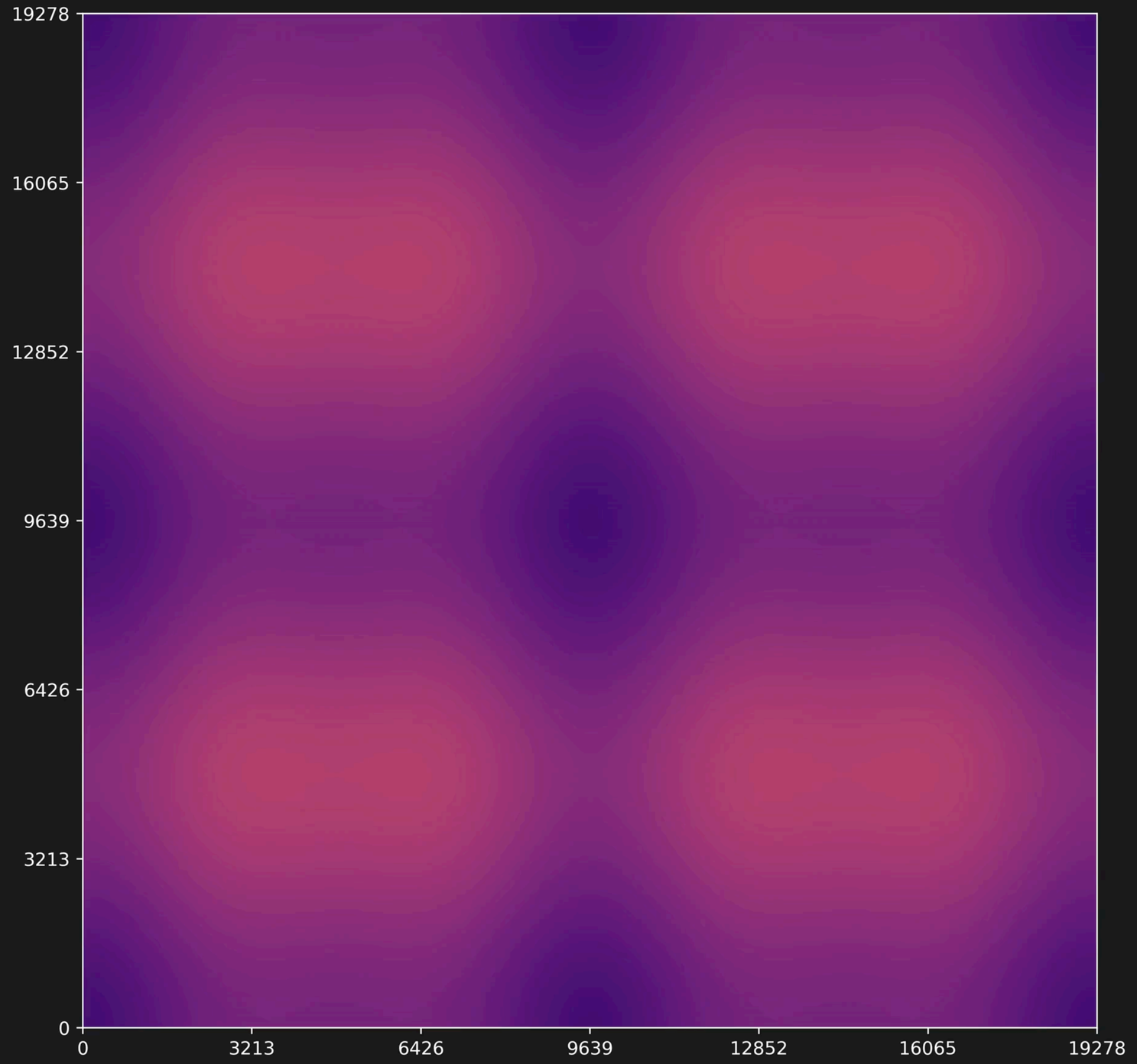
ORSZAG–TANG VORTEX

ENERGY



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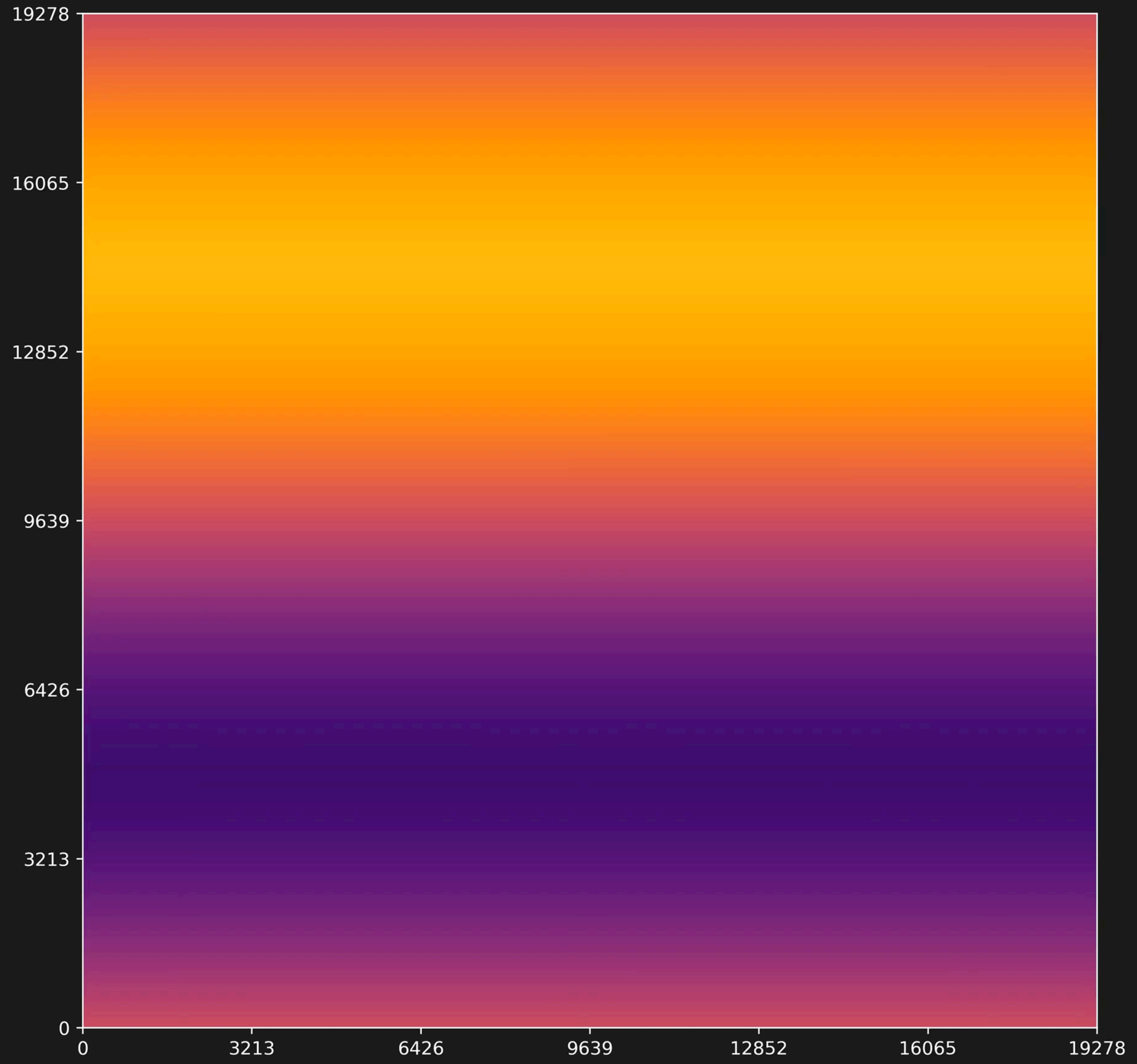
ORSZAG–TANG VORTEX

P_x



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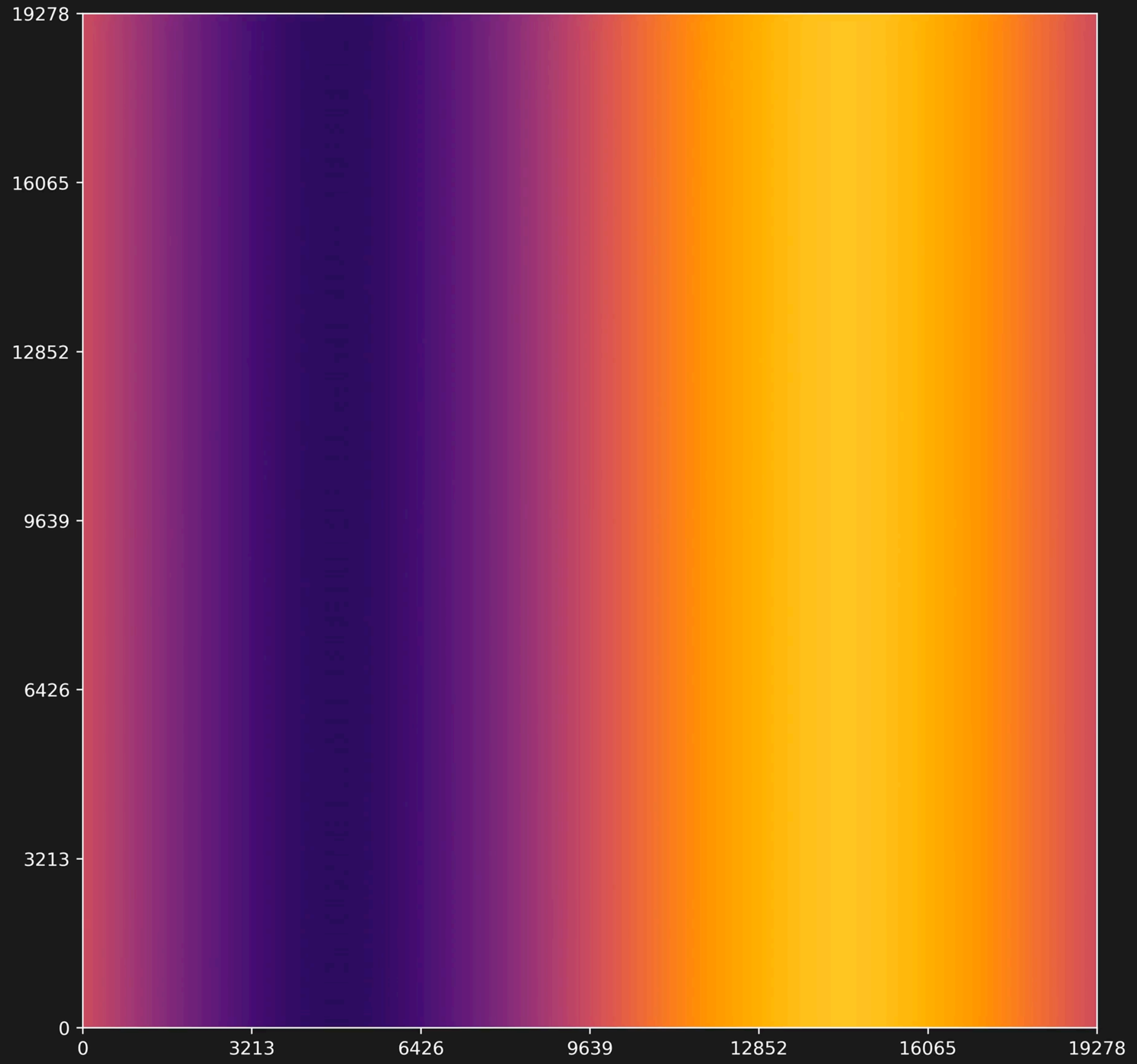
ORSZAG–TANG VORTEX

P_y



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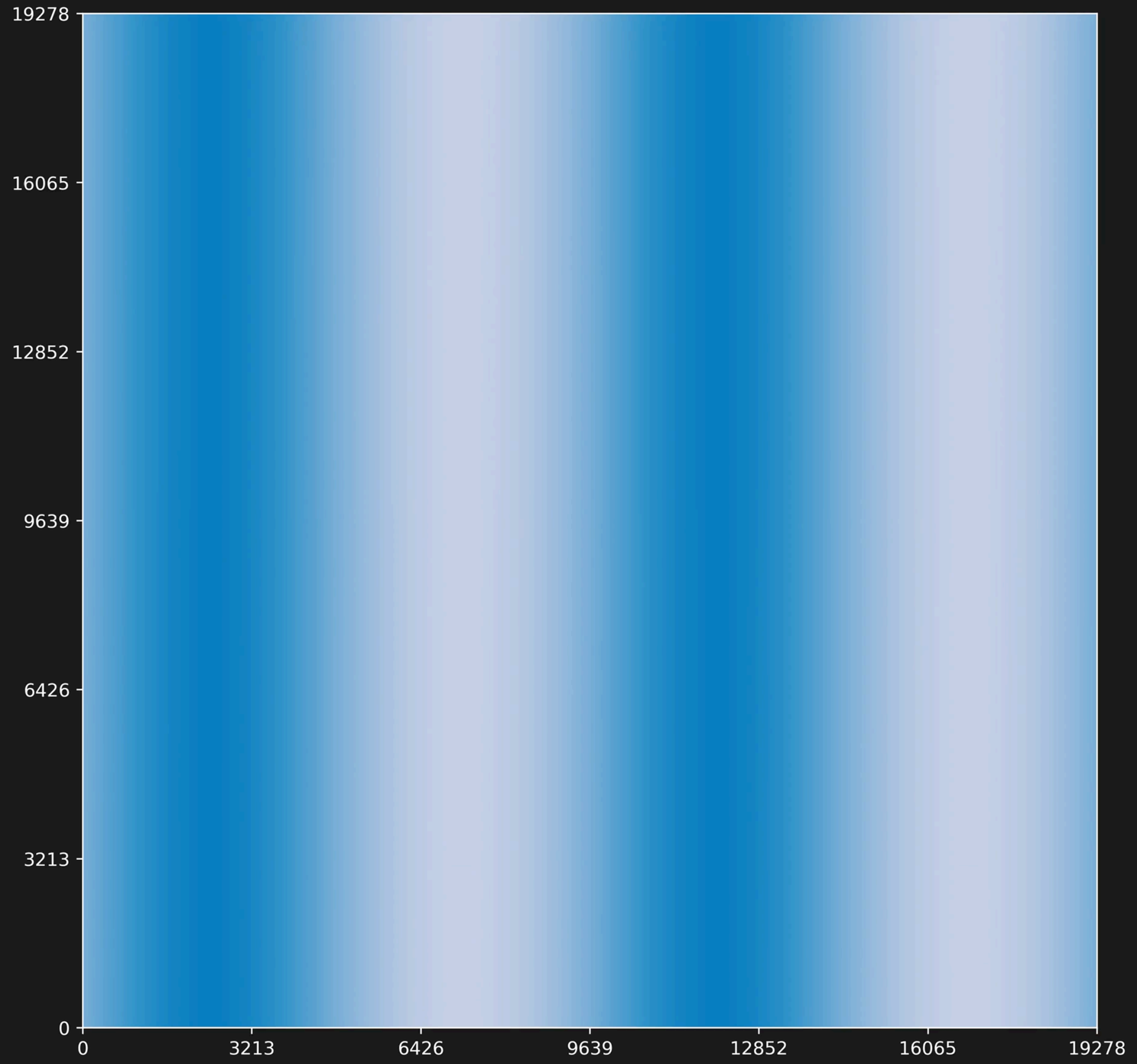
ORSZAG–TANG VORTEX

B_y



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