EXASCALE MHD SIMULATIONS WITH Cholla

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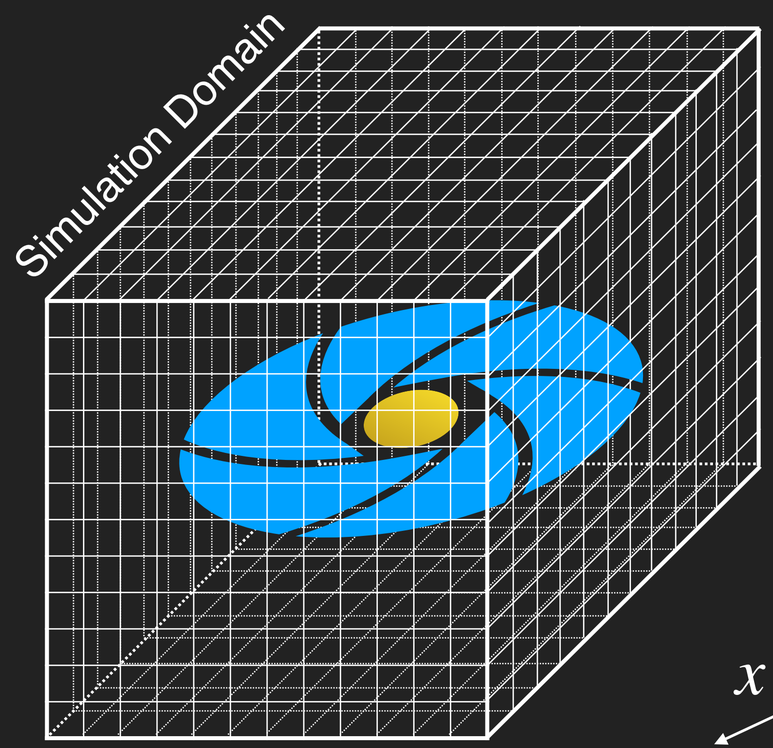
Advisor: Professor Evan Schneider

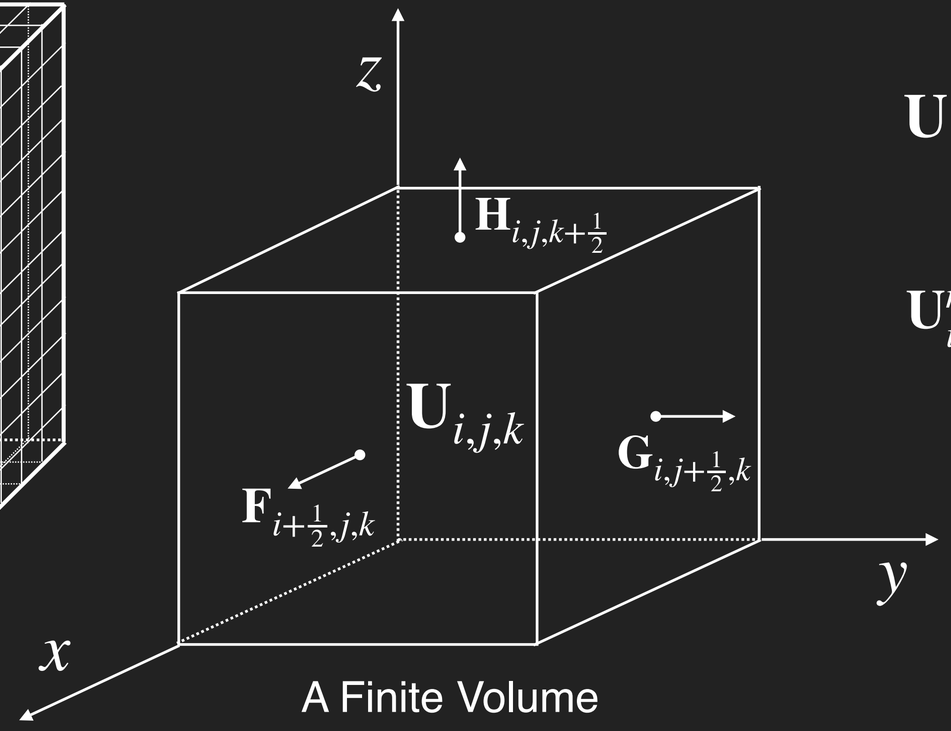
Other Graduate Students: Orlando Warren, Helena Richie

DISCLAIMER

In large part this will be a talk about software development.

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



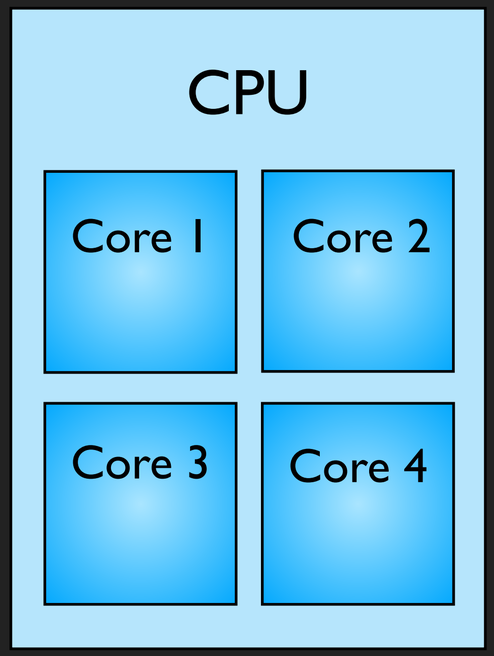


A Finite Volume

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

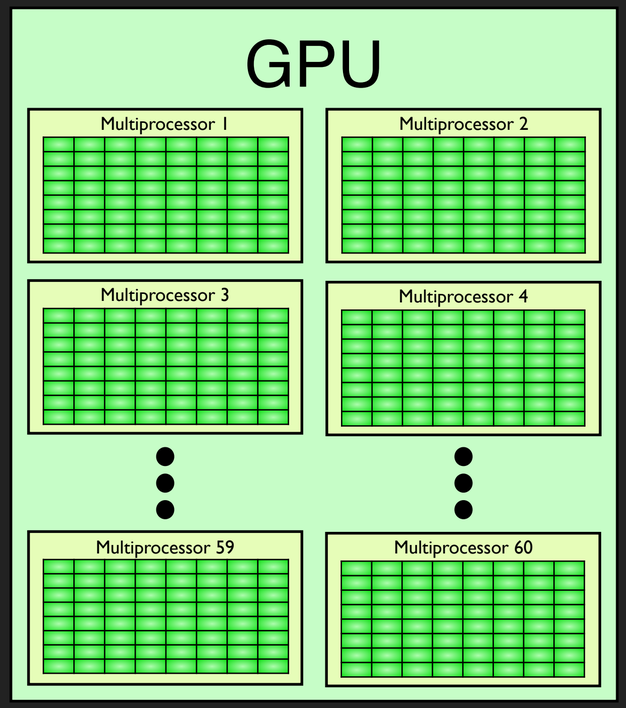
$$\mathbf{U}_{i,j,k}^{n+1} = \mathbf{U}_{i,j,k}^{n} - \frac{\delta t}{\delta x}\left(\mathbf{F}_{i+\frac{1}{2},j,k} - \mathbf{F}_{i-\frac{1}{2},j,k}\right) - \frac{\delta t}{\delta y}\left(\mathbf{G}_{i,j+\frac{1}{2},k} - \mathbf{G}_{i,j-\frac{1}{2},k}\right) - \frac{\delta t}{\delta z}\left(\mathbf{H}_{i,j,k+\frac{1}{2}}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

WHY GPUs?



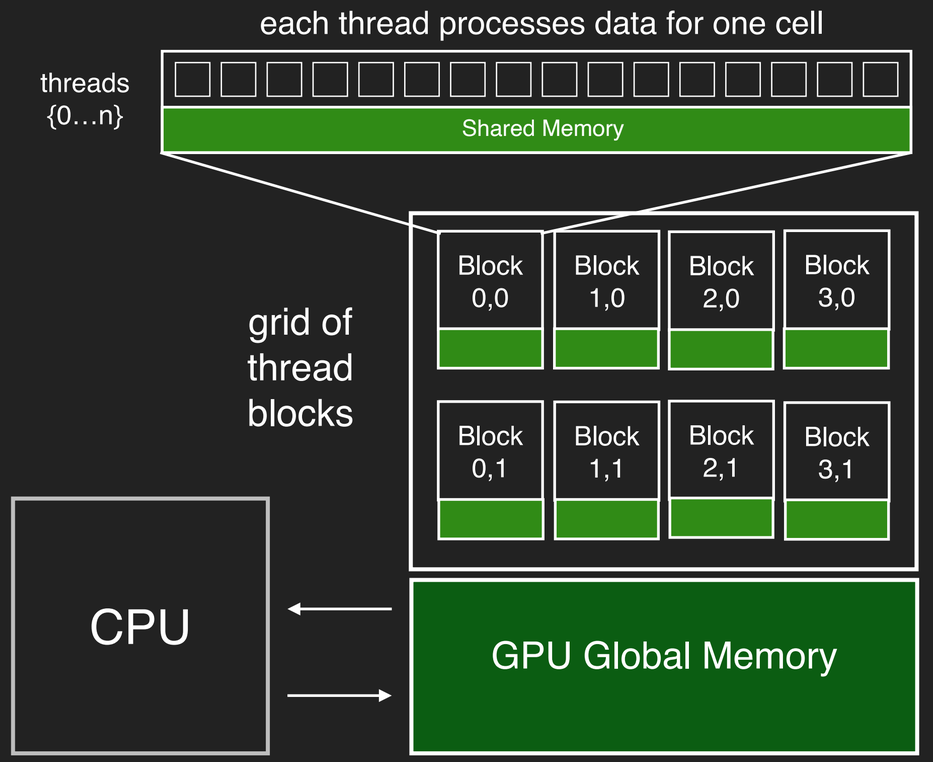
Optimized for Serial Tasks

~1-2 TFLOPS
≤128 cores
~4 GFLOPS/Watt

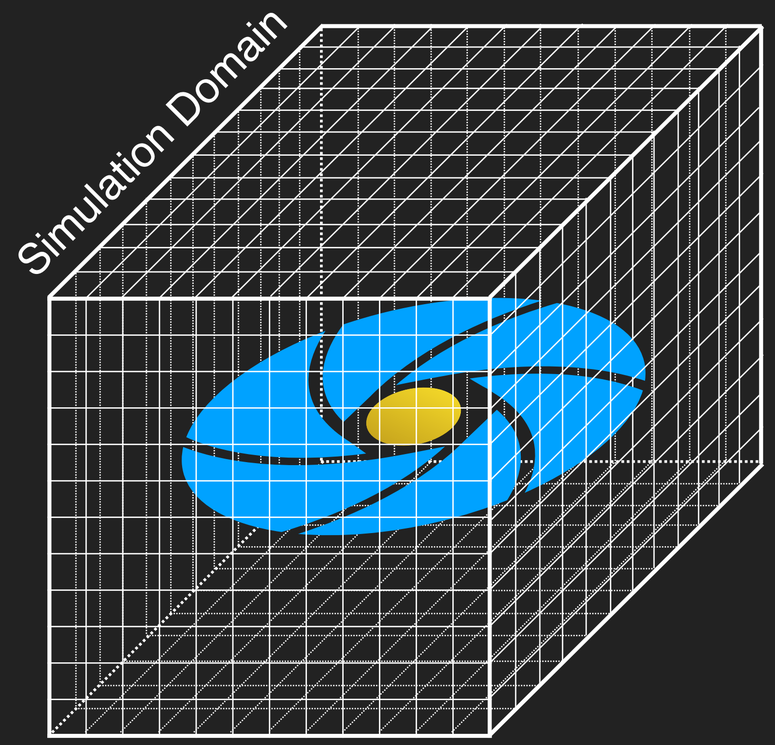


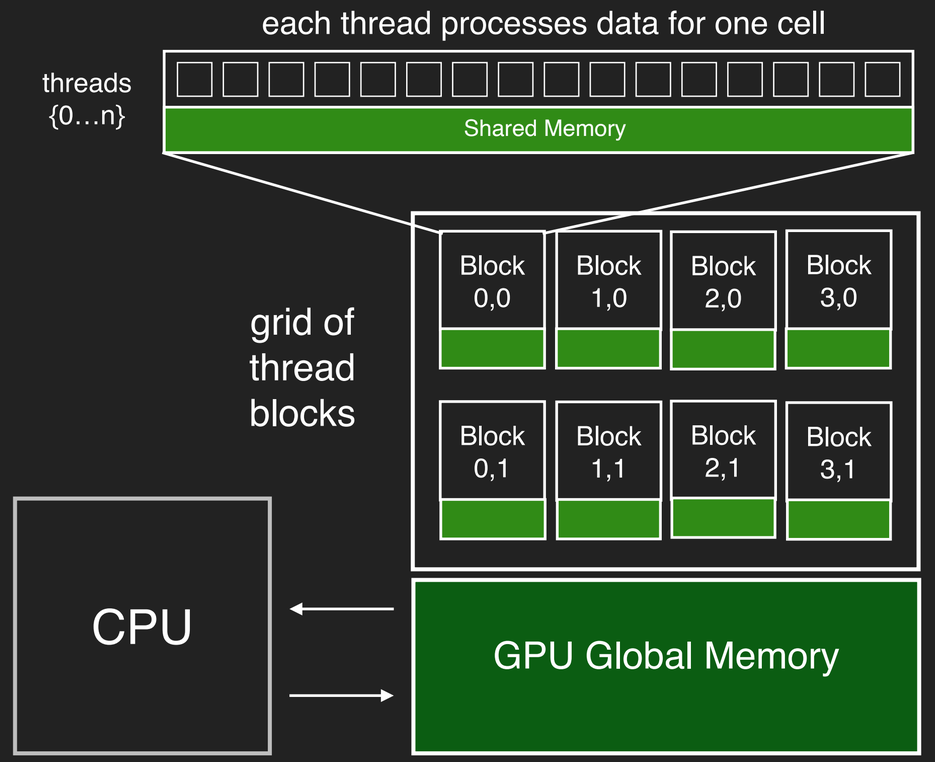
Optimized for Parallel Tasks

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



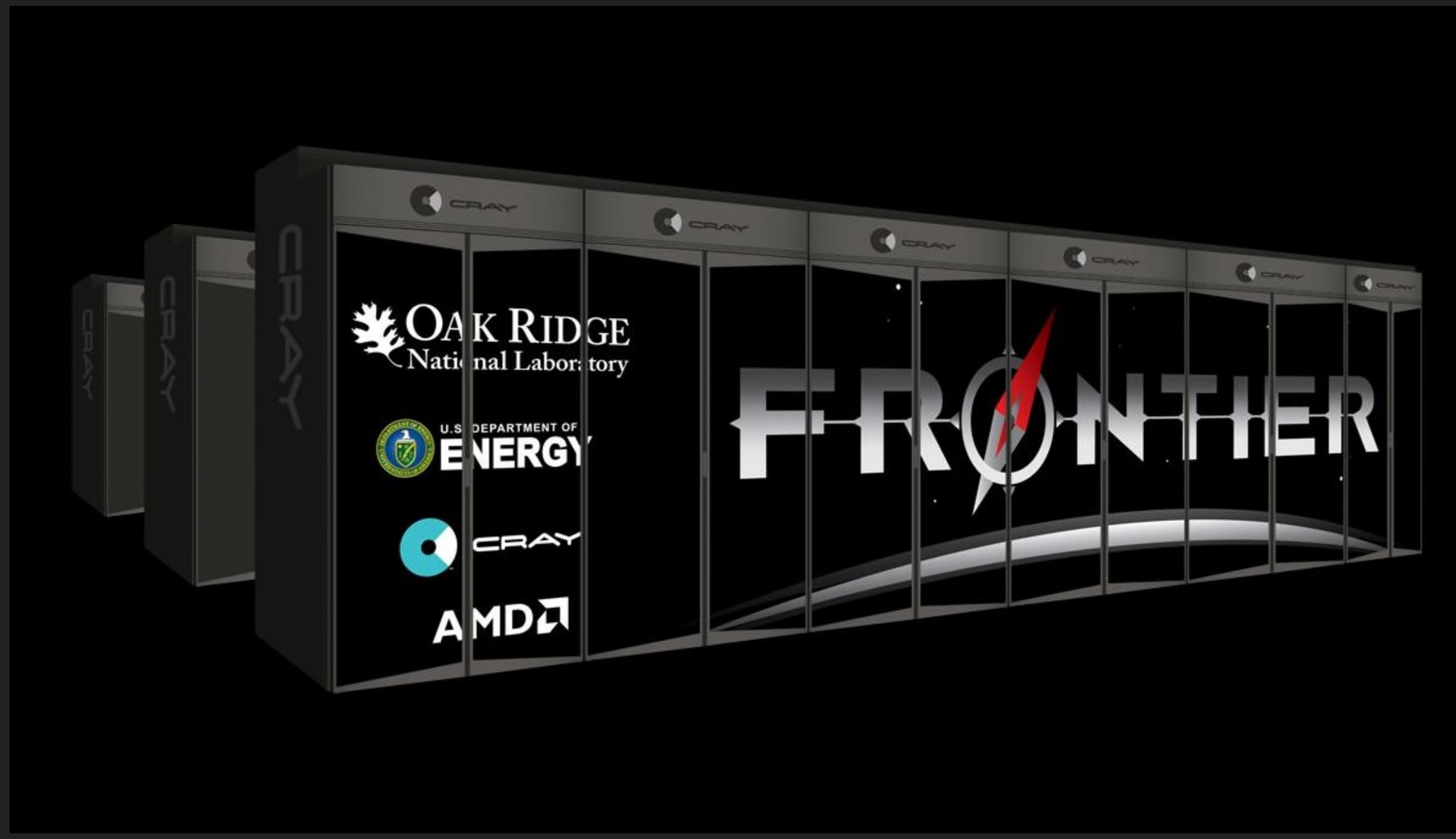
WHY GPUs?


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

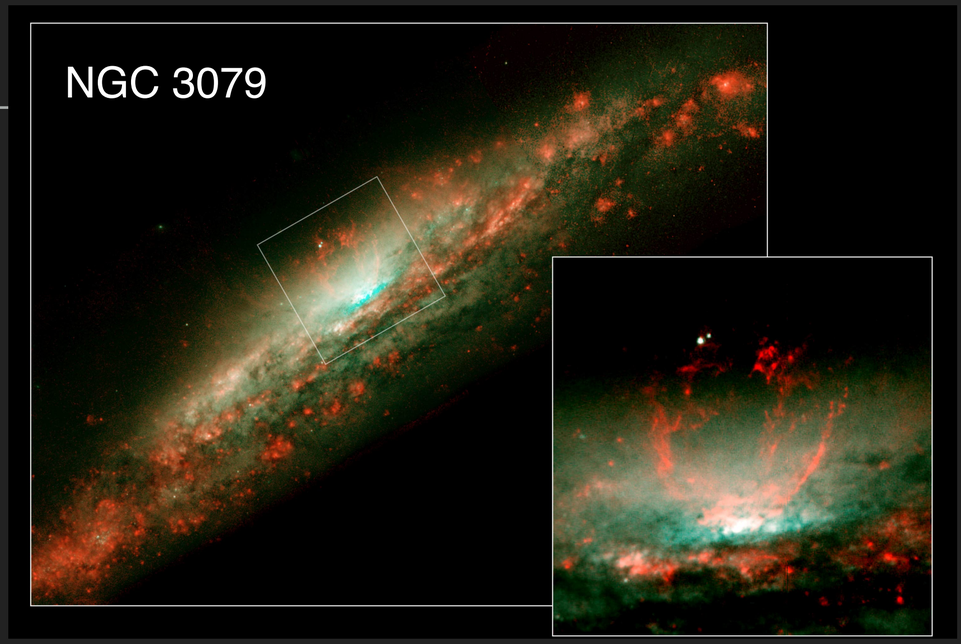
FRONTIER – EXASCALE SUPERCOMPUTERS

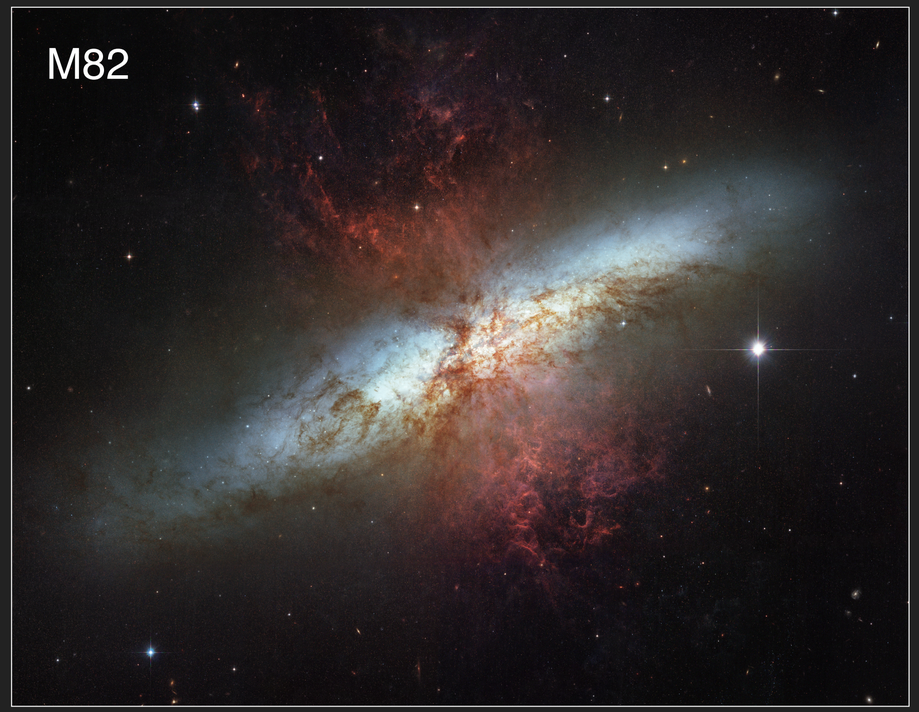
- *Frontier*, at Oak Ridge National Lab, topped the HPC top500 list on June 1, 2022.
  - 1.1 EF - 1.5 EF
  - 1 AMD EPYC CPU & 4 AMD MI250X GPUs per node
  - National resource allocated through INCITE and ALCC



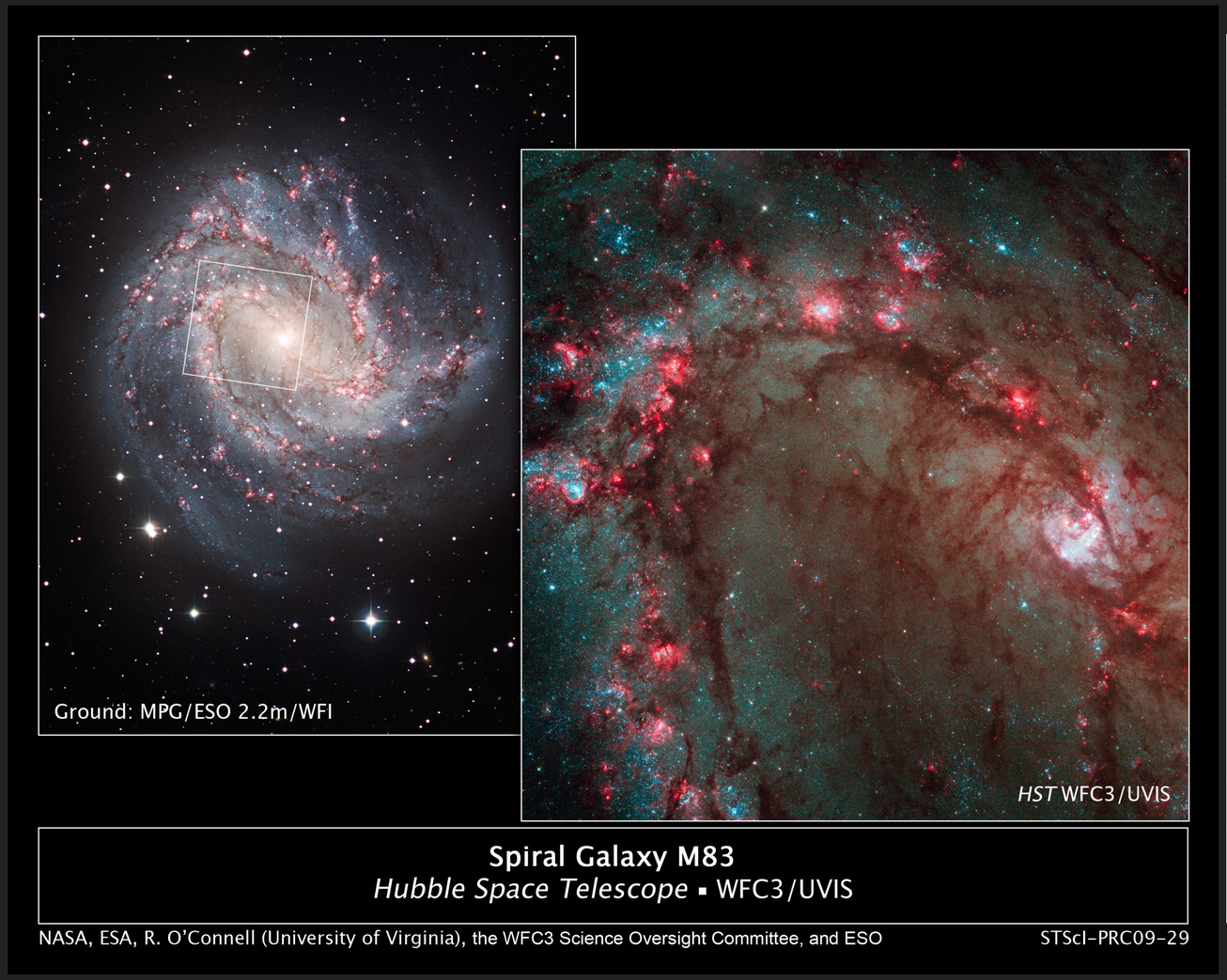
THE UBIQUITY OF OUTFLOWS

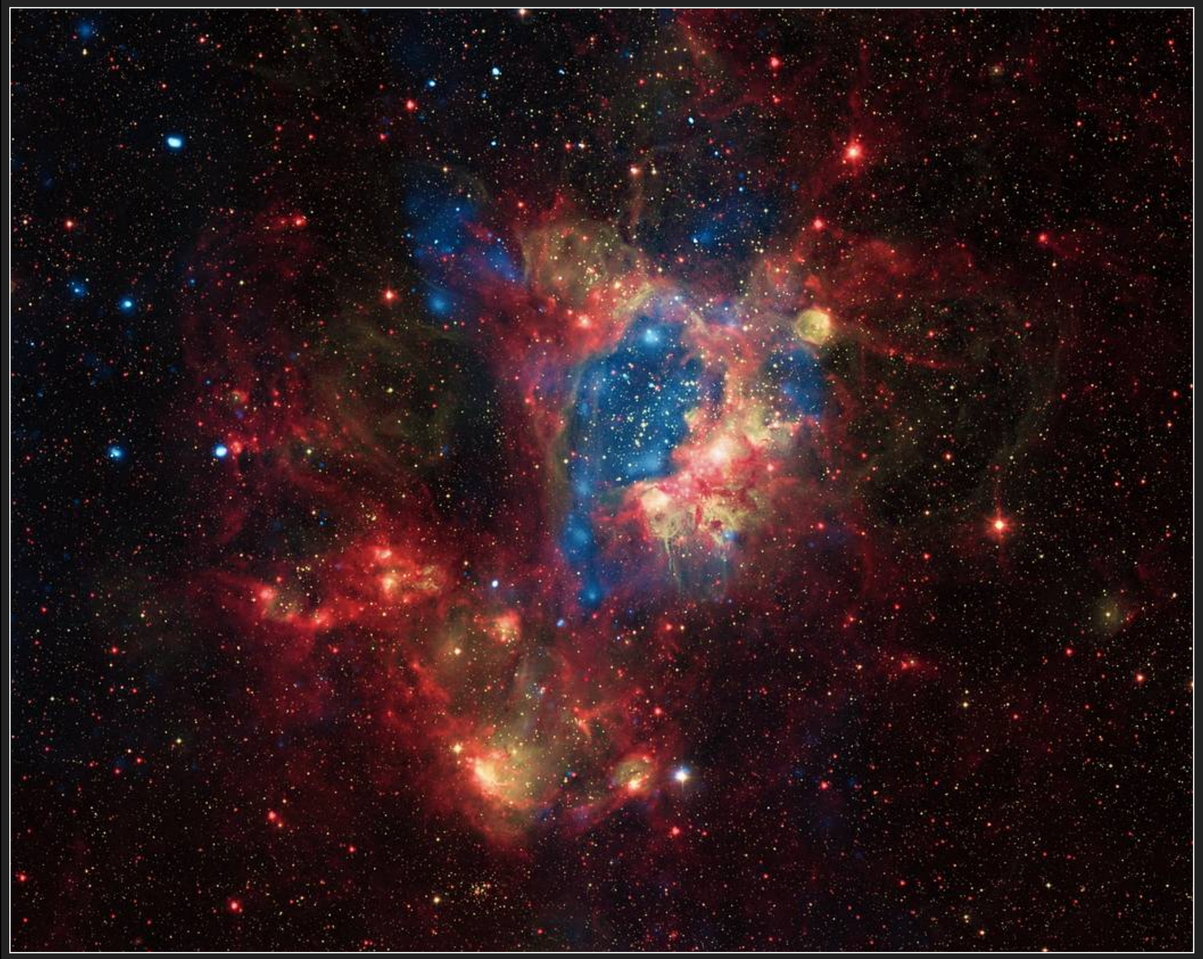
- Local star-forming galaxies are routinely observed to host outflows.
- At higher redshift, the incidence rate of observed outflows increases (e.g. Rubin 2014).
- Data are consistent with all galaxies driving outflows at various points in their lives.
- We want to understand this process!



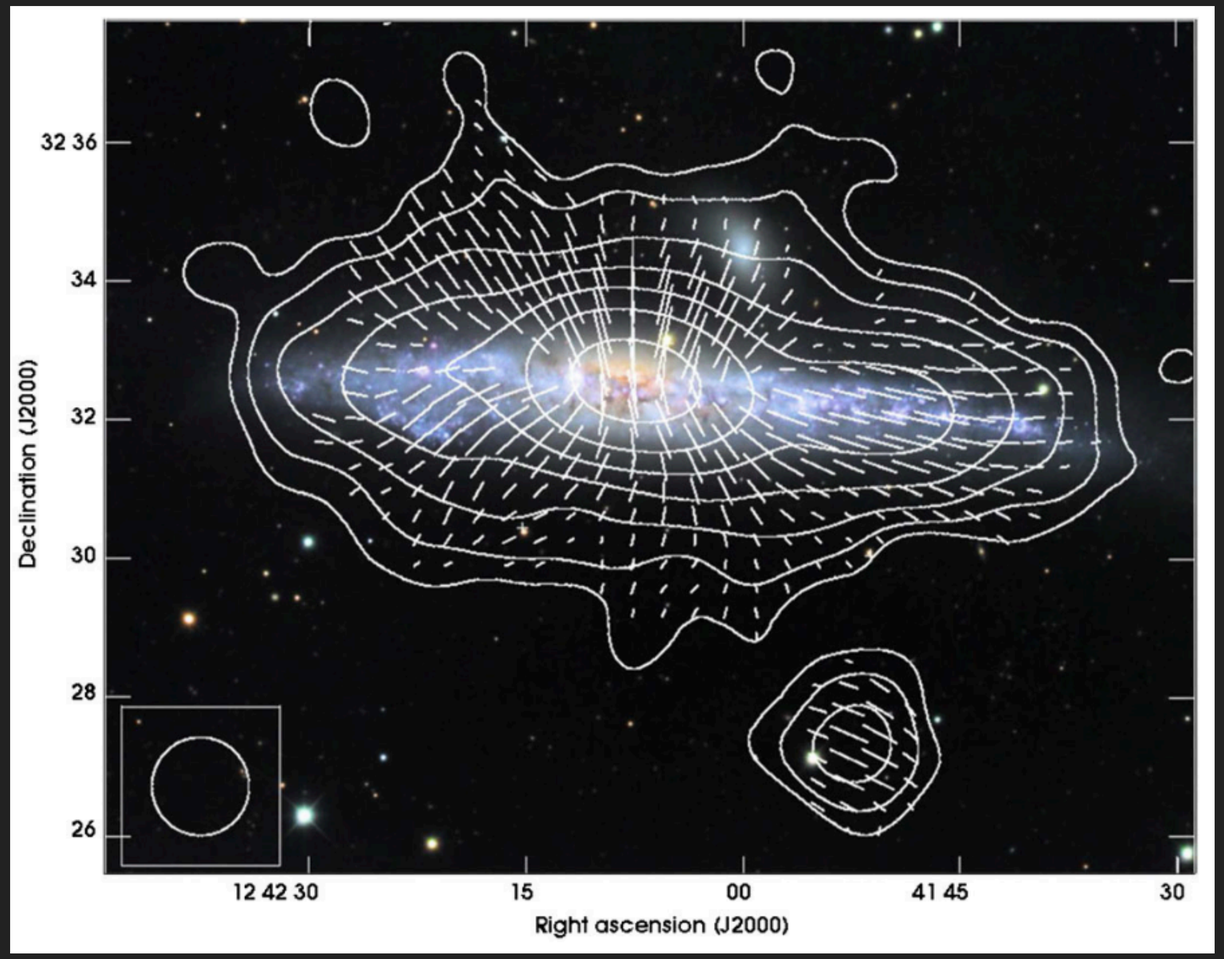


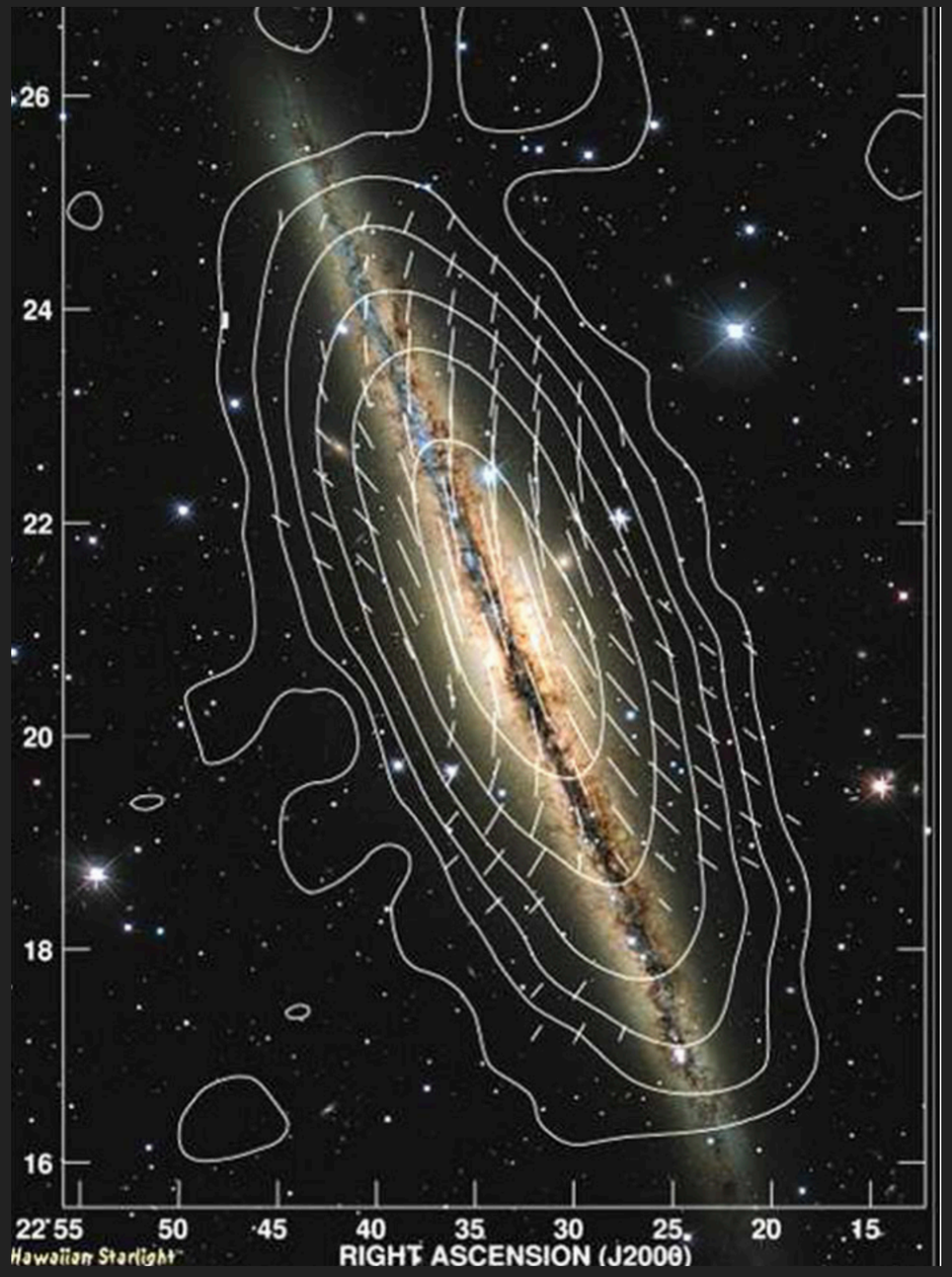
THE CHALLENGE – PARSEC SCALES – STELLAR FEEDBACK





THE CHALLENGE – PARSEC SCALES – MAGNETIC FIELDS



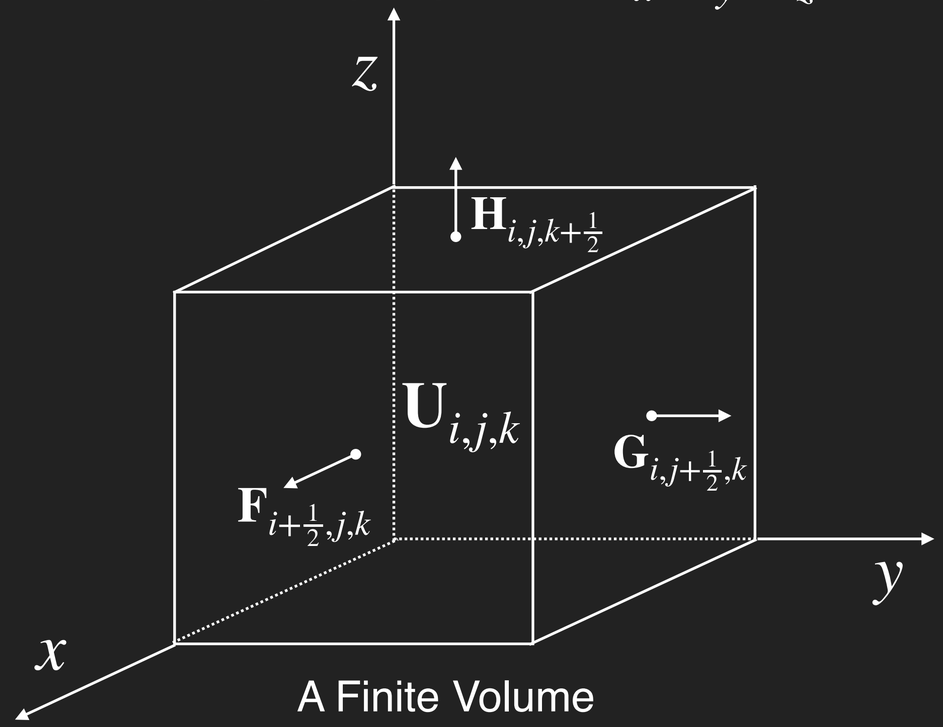


QUESTIONS?

HOW TO REPRESENT THE MAGNETIC FIELD?

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

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

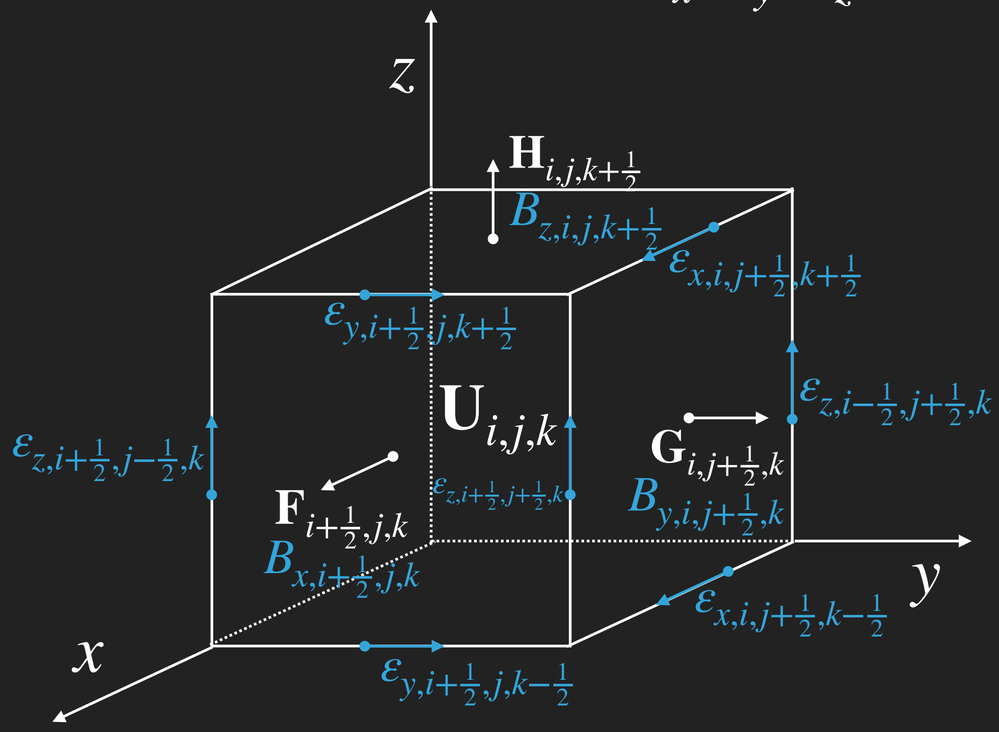


A Finite Volume

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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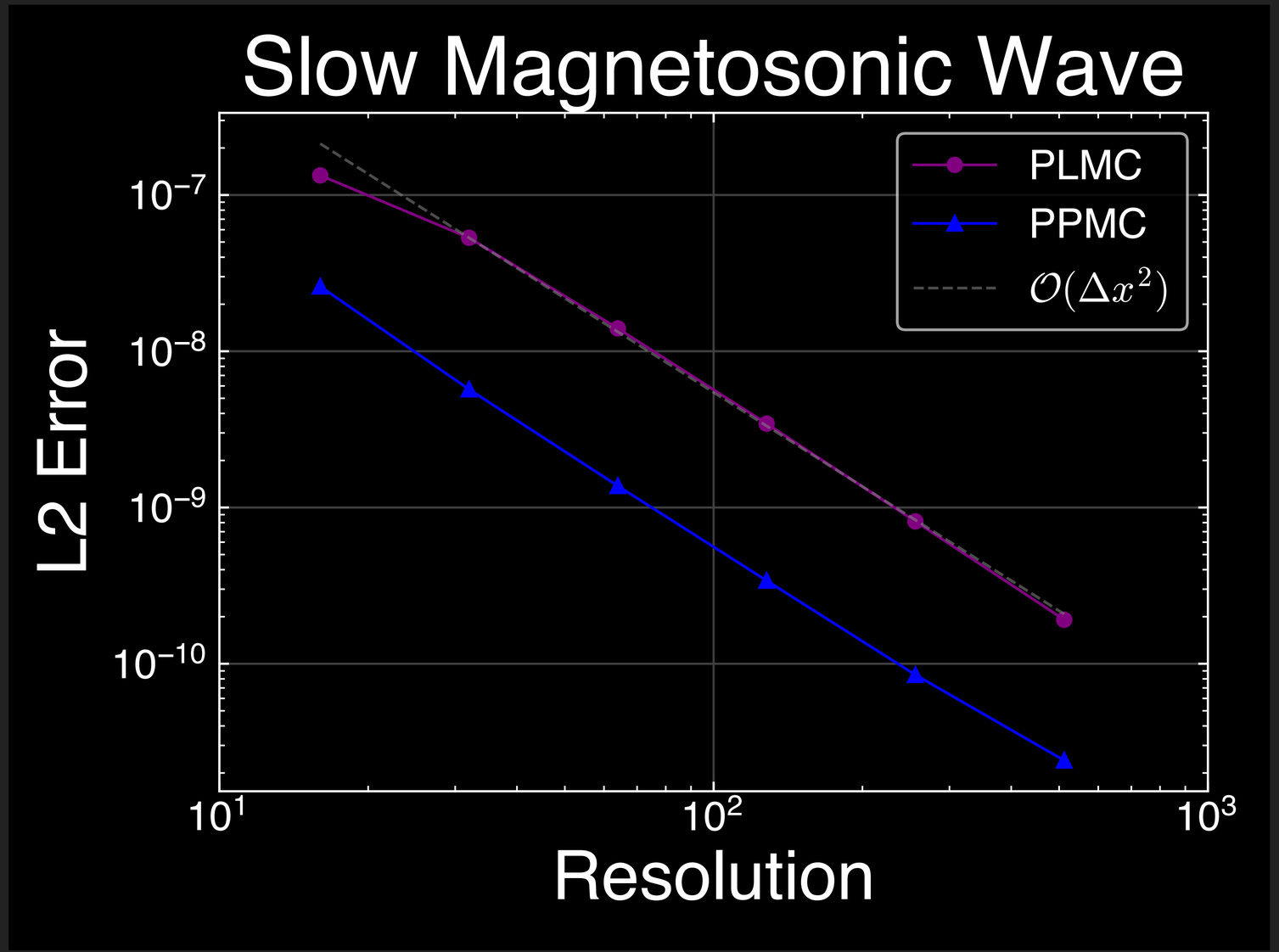
LINEAR WAVE CONVERGENCE



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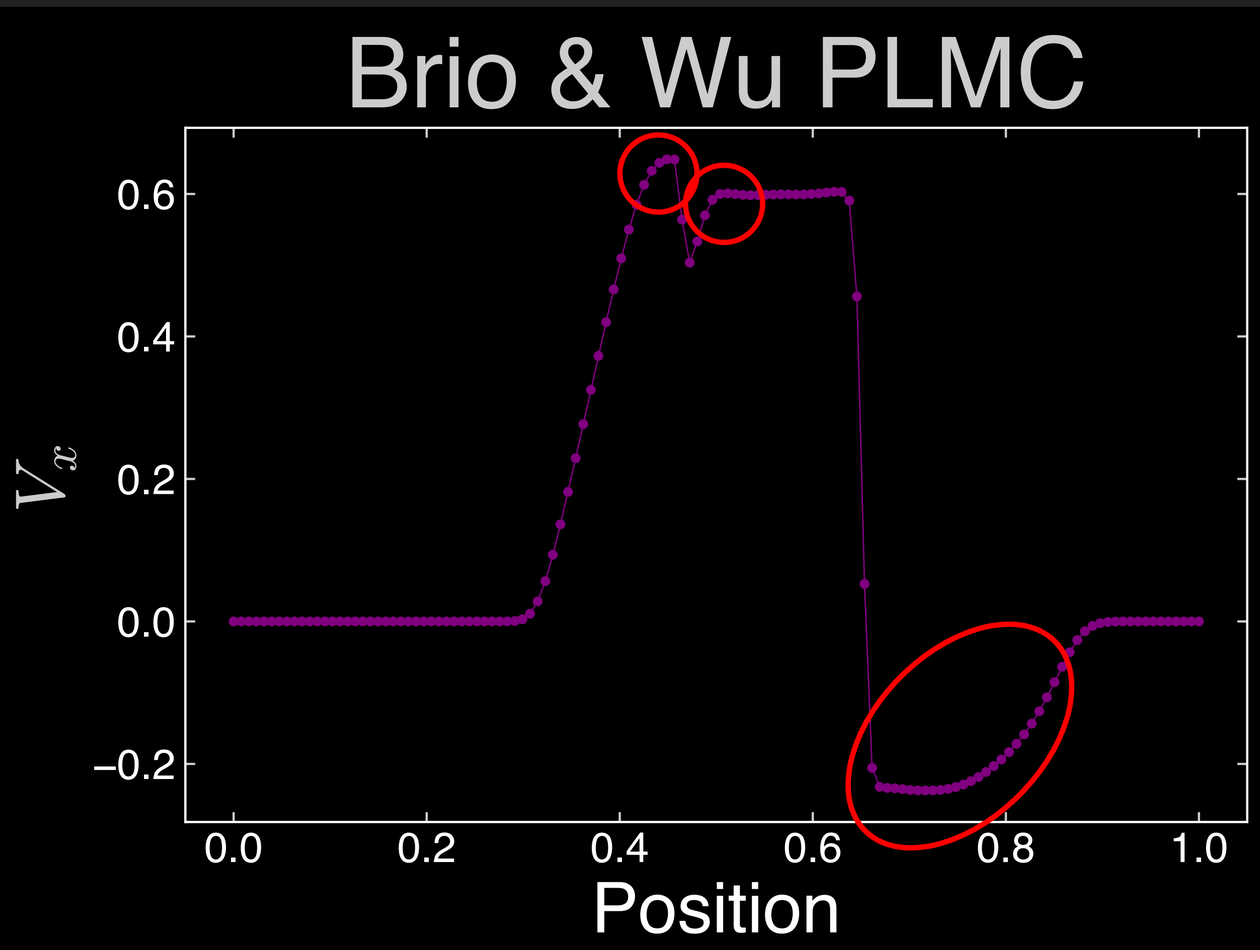
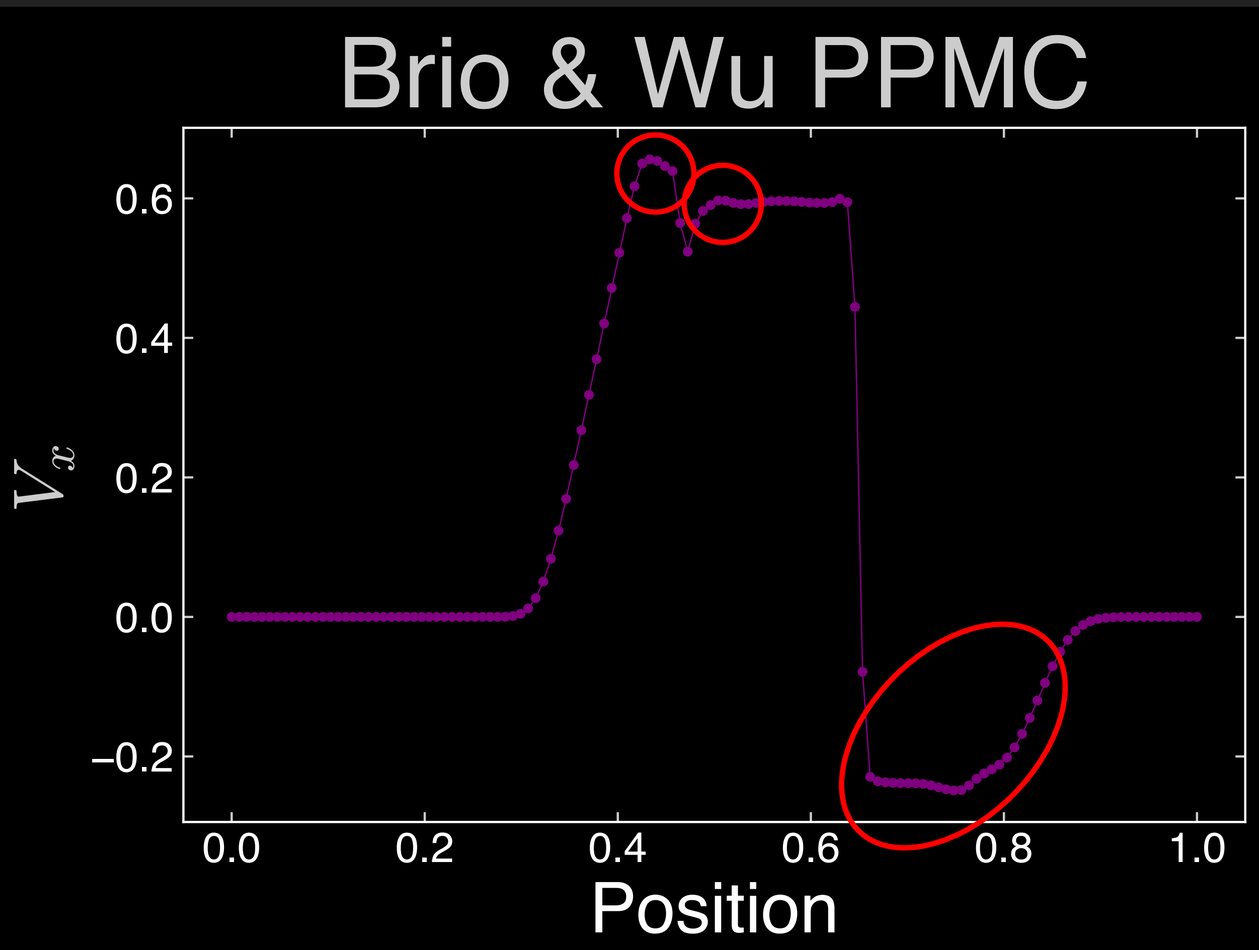
PPMC VS. PLMC – SHOCKS





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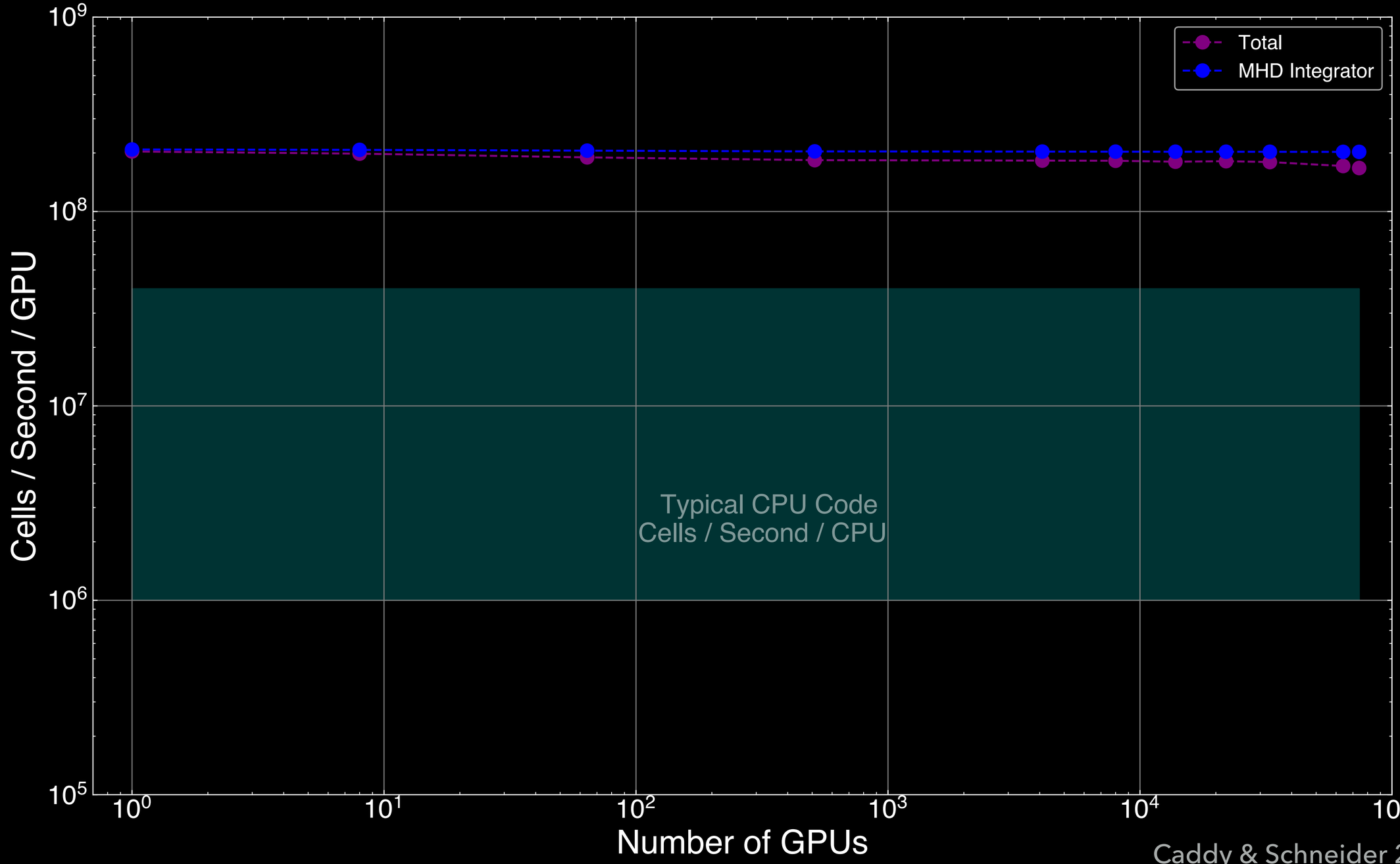
MHD Weak Scaling on Frontier (PLMC)



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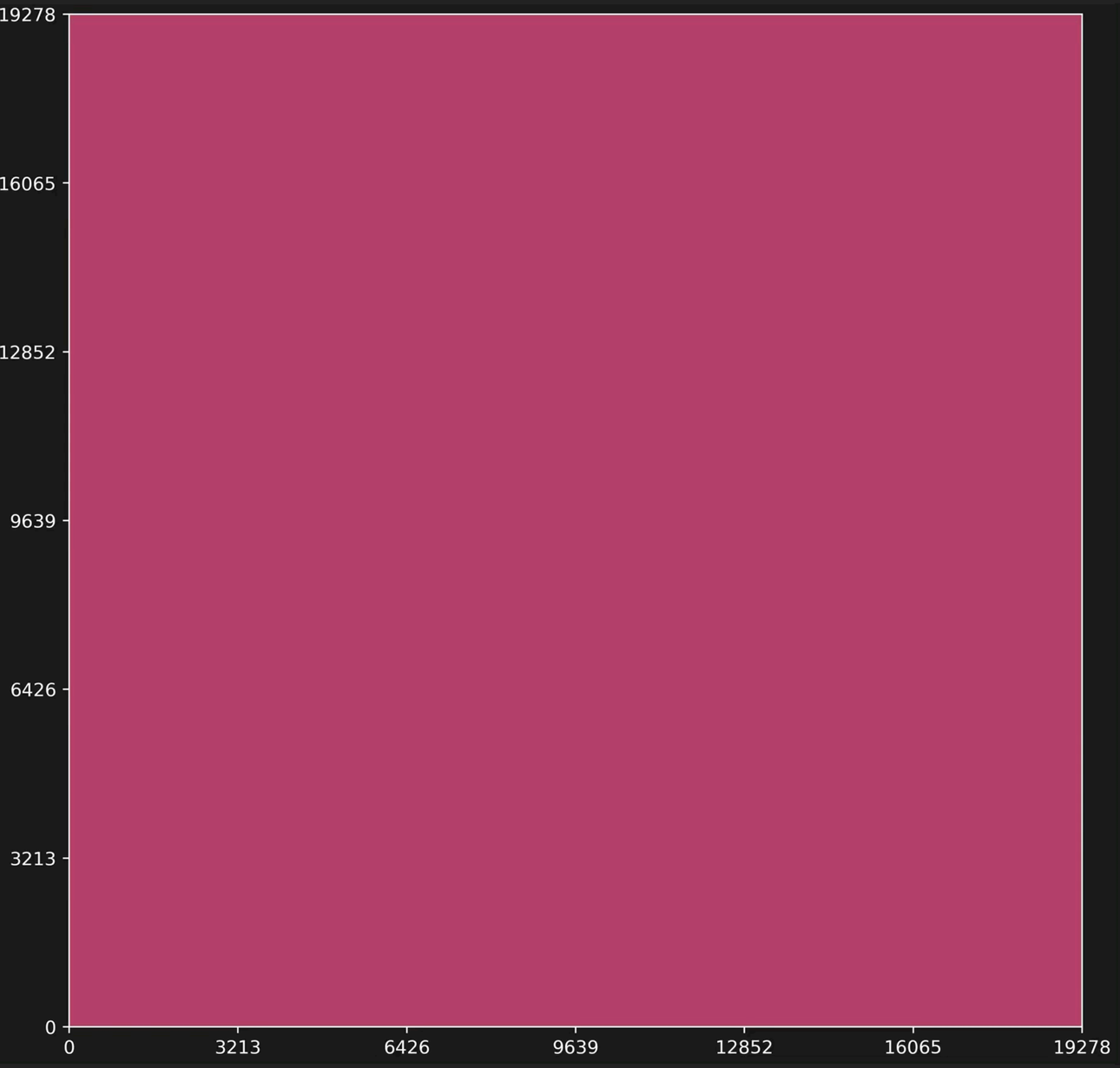
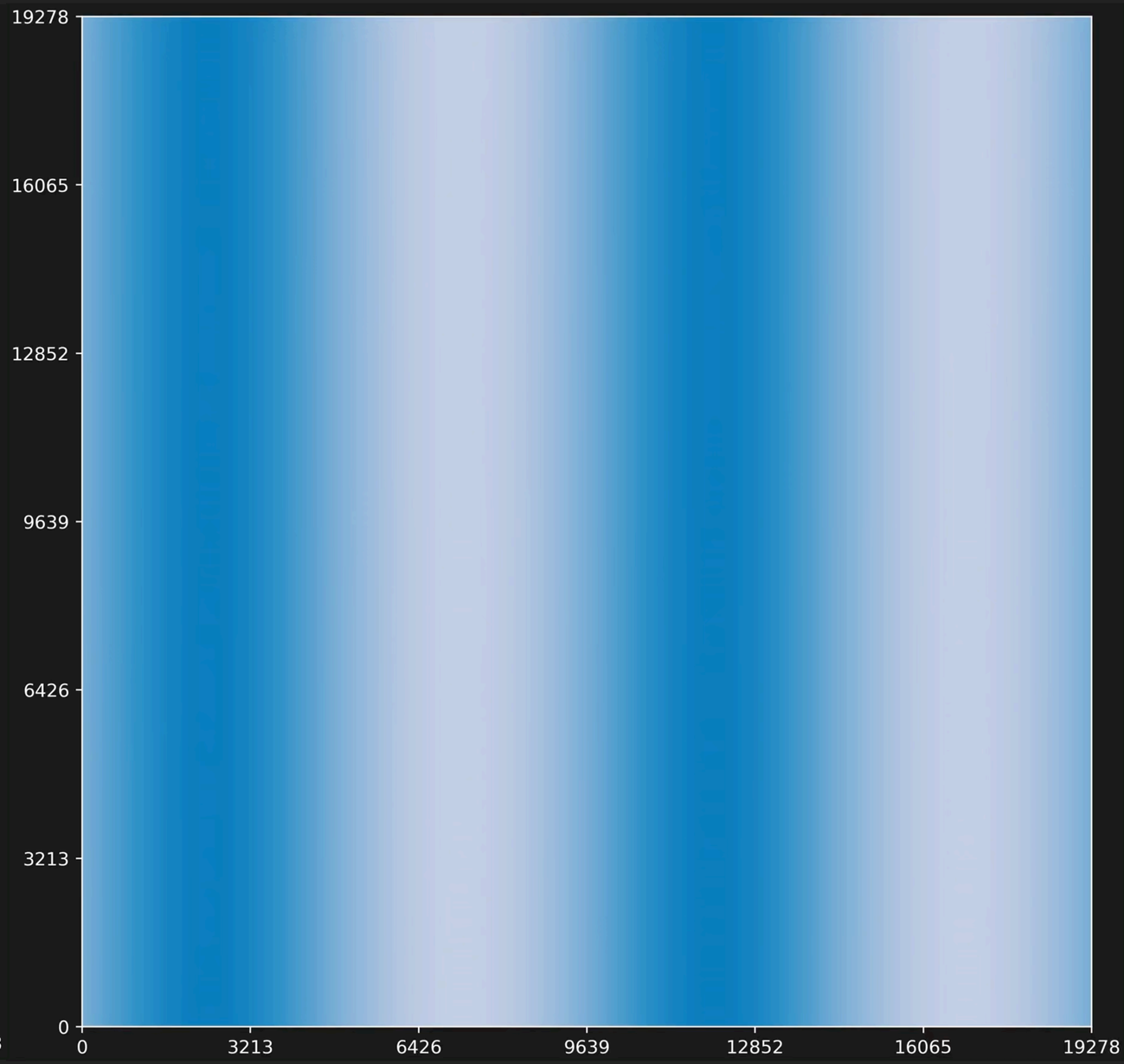
DENSITY

ORSZAG-TANG VORTEX

B_x





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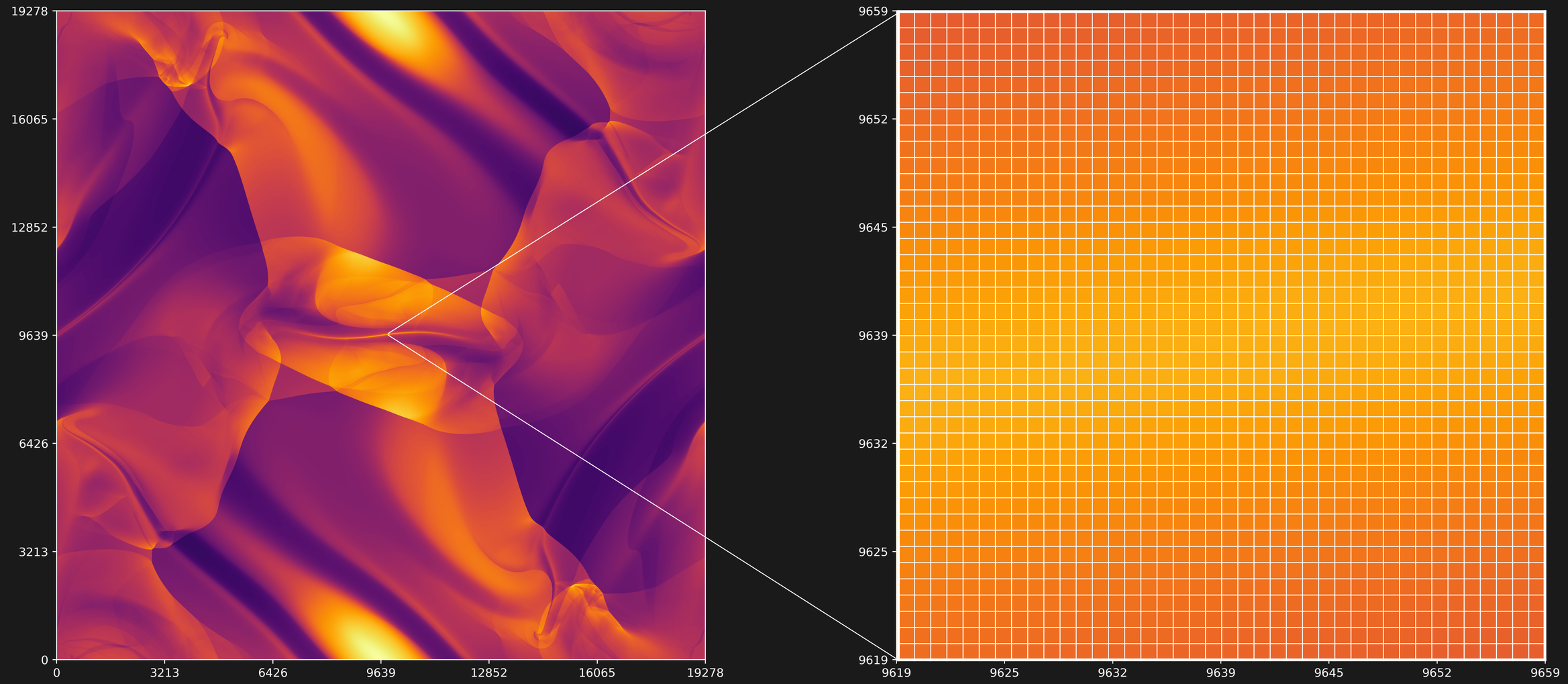
19278
16065
12852
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6426
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19278
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9645
9639
9632
9625
9619
9619
9625
9632
9639
9645
9652
9659

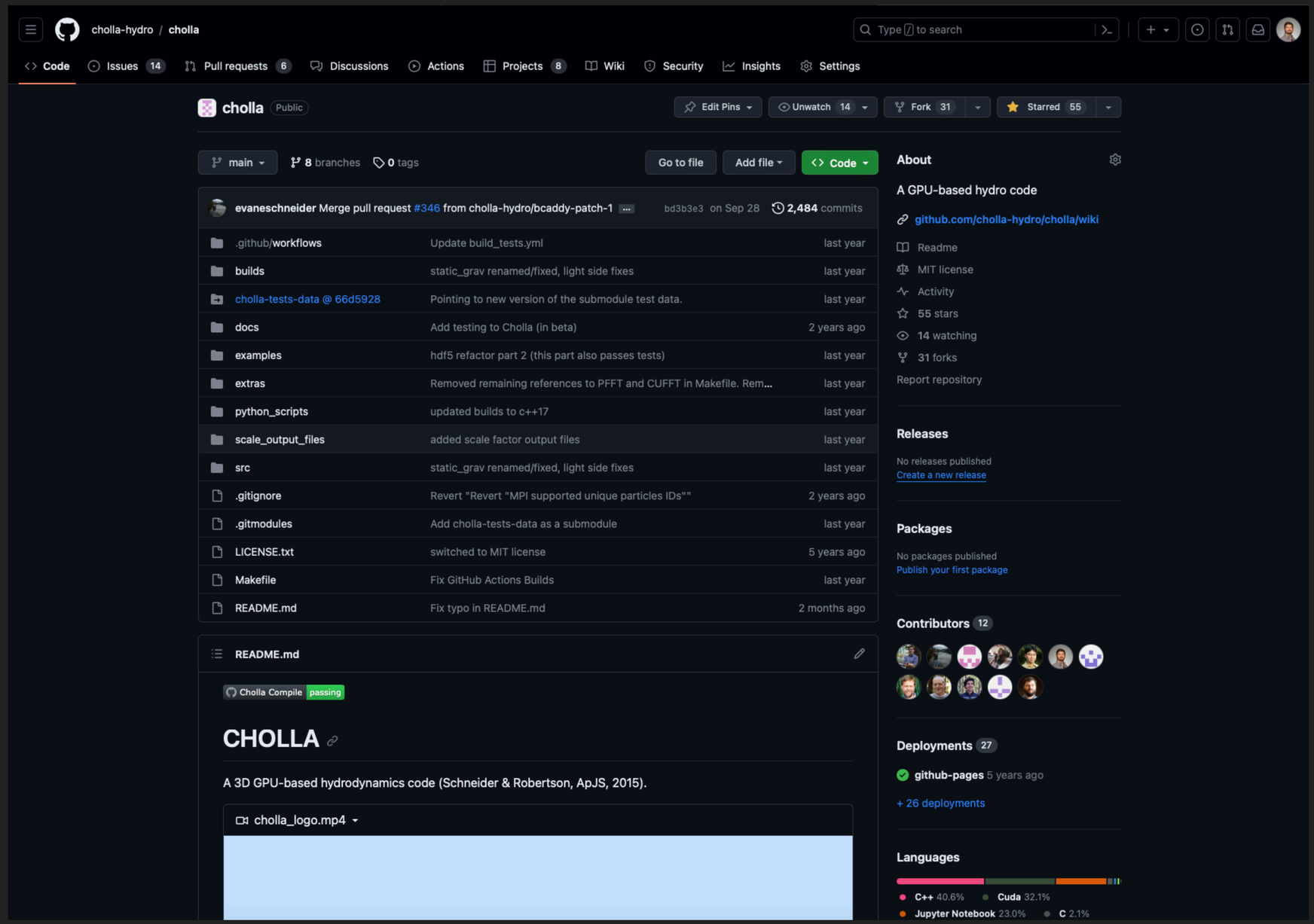
QUESTIONS?

MOTIVATIONS

- Correctness
  - Improve the quality and accuracy of the code
  - Rigorous science needs reproducibility and reasonable proof of correctness
- Invested Time
  - Best Practices reduce errors and make code faster and easier to work with
  - Invested time is paid back in time savings later
- Usually a social rather than technical problem

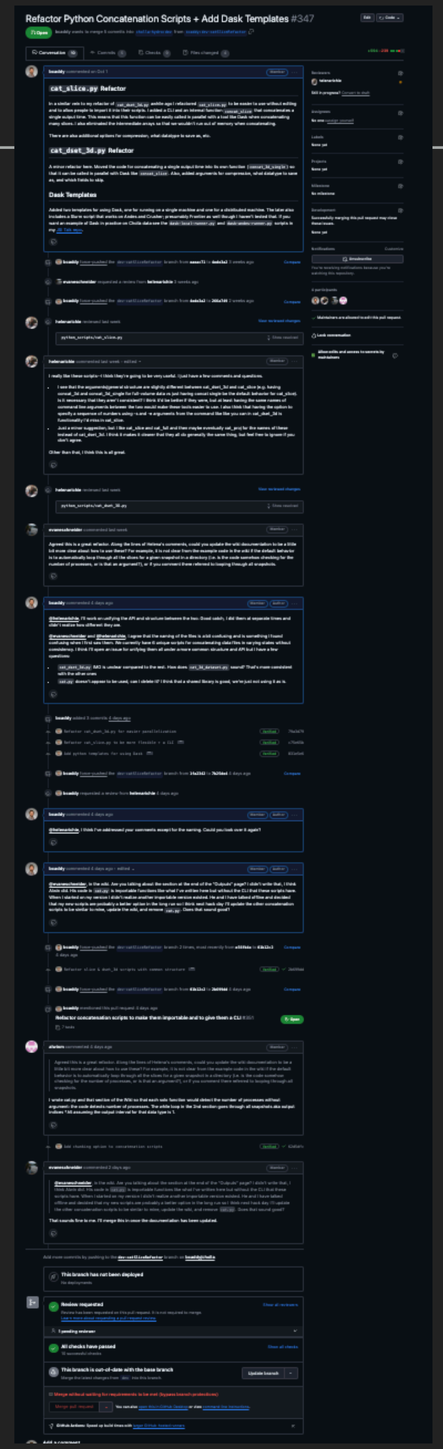
VERSION CONTROL

- Enables collaboration
- Reproducibility
- Revert errors
- Backup
- Providers (GitHub, GitLab, etc) have good tools, use them



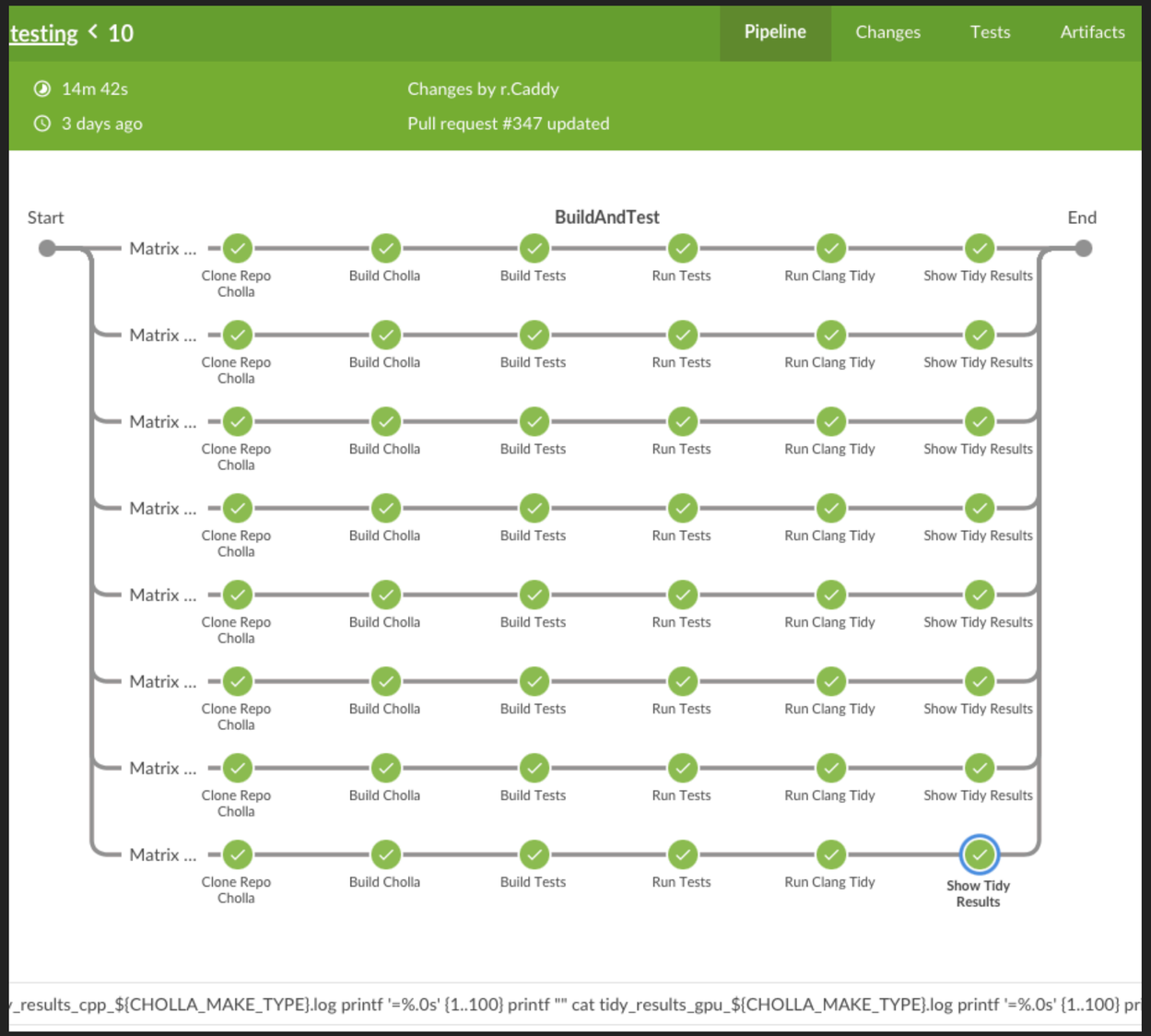
CODE REVIEWS

- Have someone else look at your code
- Catches a lot of minor issues and major ones
- Knowledge transfer
- Positive peer pressure to improve code quality
- Improve sense of community



TESTING + AUTOMATED TESTING

- 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)



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STATIC ANALYZER

- Examines code without executing, uncovering errors, vulnerabilities, and quality issues early.
- Improves reliability, debugging, and maintainability.
- In our code:
  - Found several minor bugs
  - Reduced the complexity of many sections of code
  - Guided us in entirely removing all C code
  - Automated in every PR

```
int n_cells = nx * ny * nz;
int o1, o2, o3;
if (dir = 0) {    an assignment within an 'if' condition is bug-prone
  o1 = 1;
  o2 = 2;
  o3 = 3;
}
if (dir == 1) {
  o1 = 2;
  o2 = 3;
  o3 = 1;
}
if (dir == 2) {
  o1 = 3;
  o2 = 1;
  o3 = 2;
}
```

FORMATTING

- Makes code consistent
- Improves group ownership
- No need to think about formatting when writing code, let the computer do it
- Automated checking in PRs

```
0 references
table 50109 MyTable{

    fields    {
                0 references
                field(1;        MyField;        Integer){
}
        }

    0 references
    var         myInt: Integer;

    trigger OnInsert();    begin    end;
}
```

HOW DID WE DO THIS?

- I made it happen
- Group buy in when benefits quickly appeared
- Group brainstorming on next steps
- Engaging in code reviews, all code must be reviewed
- Hack days: half a day once or twice a month to work on best practices

CONCLUSION

- Cholla 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

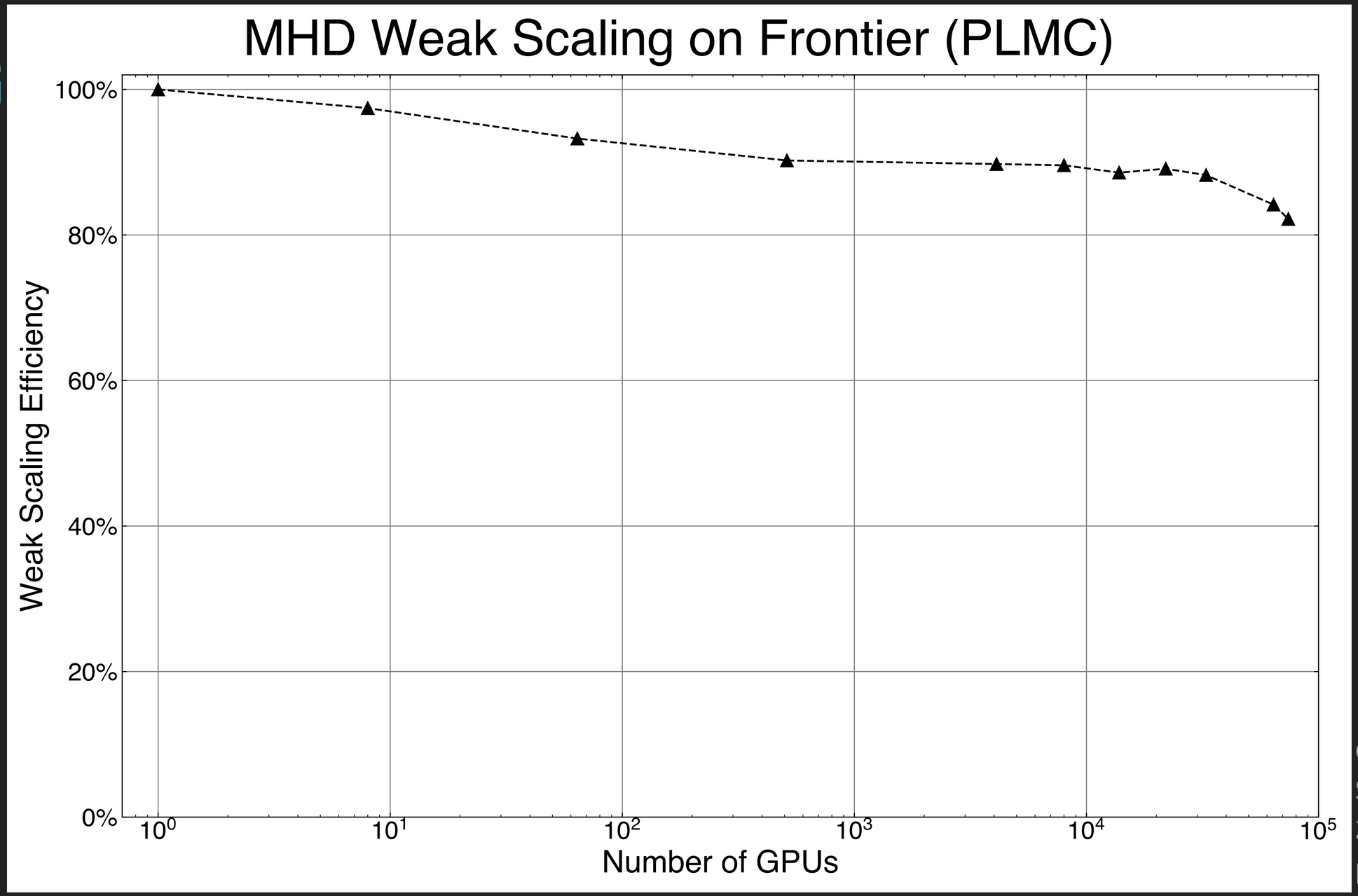
ADDITIONAL SLIDES

robertcaddy.com

github.com/bcaddy/JSI_Workshop_Talk_2023

github.com/cholla-hydro/cholla

SCALING PLOTS



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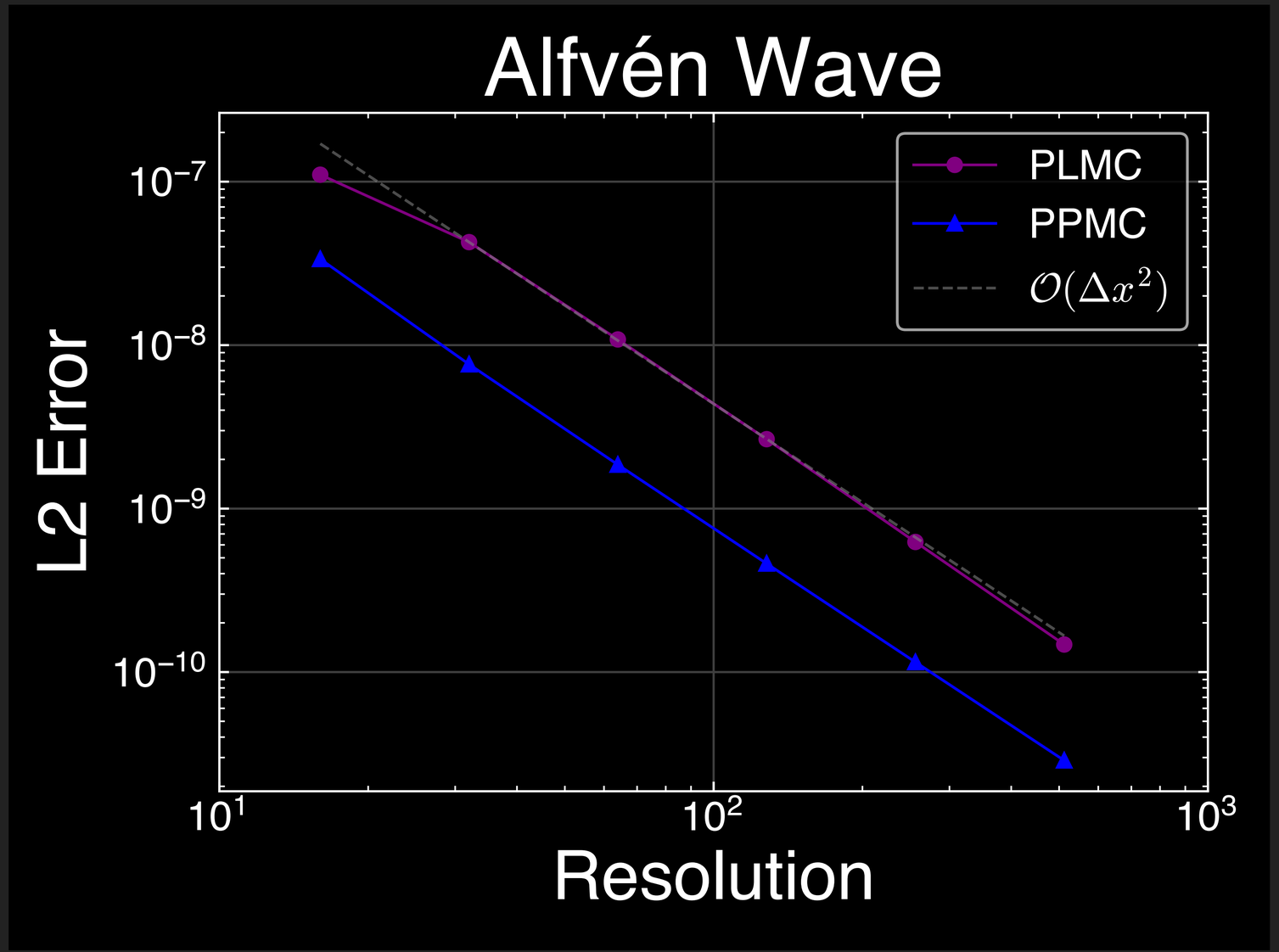

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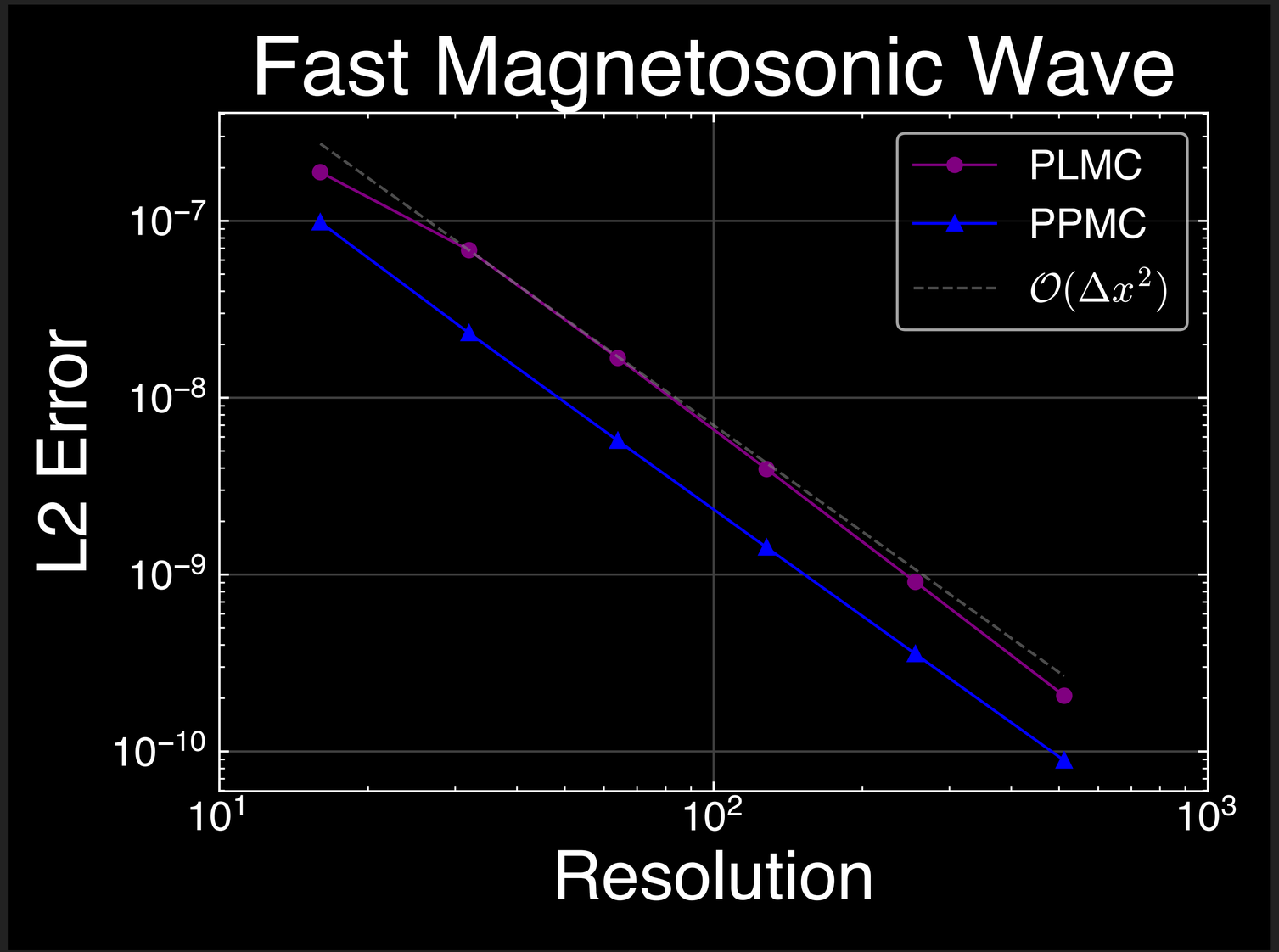

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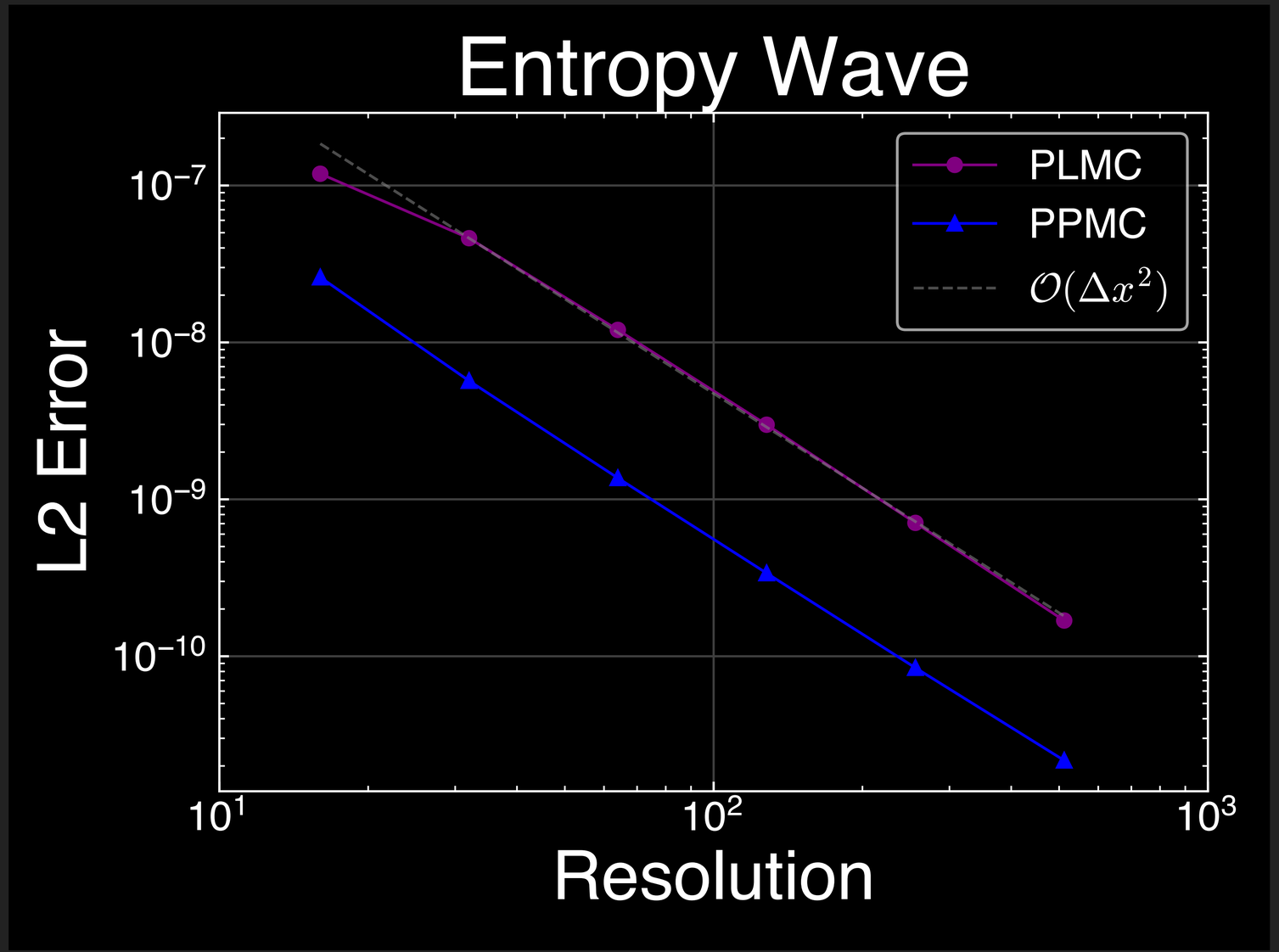

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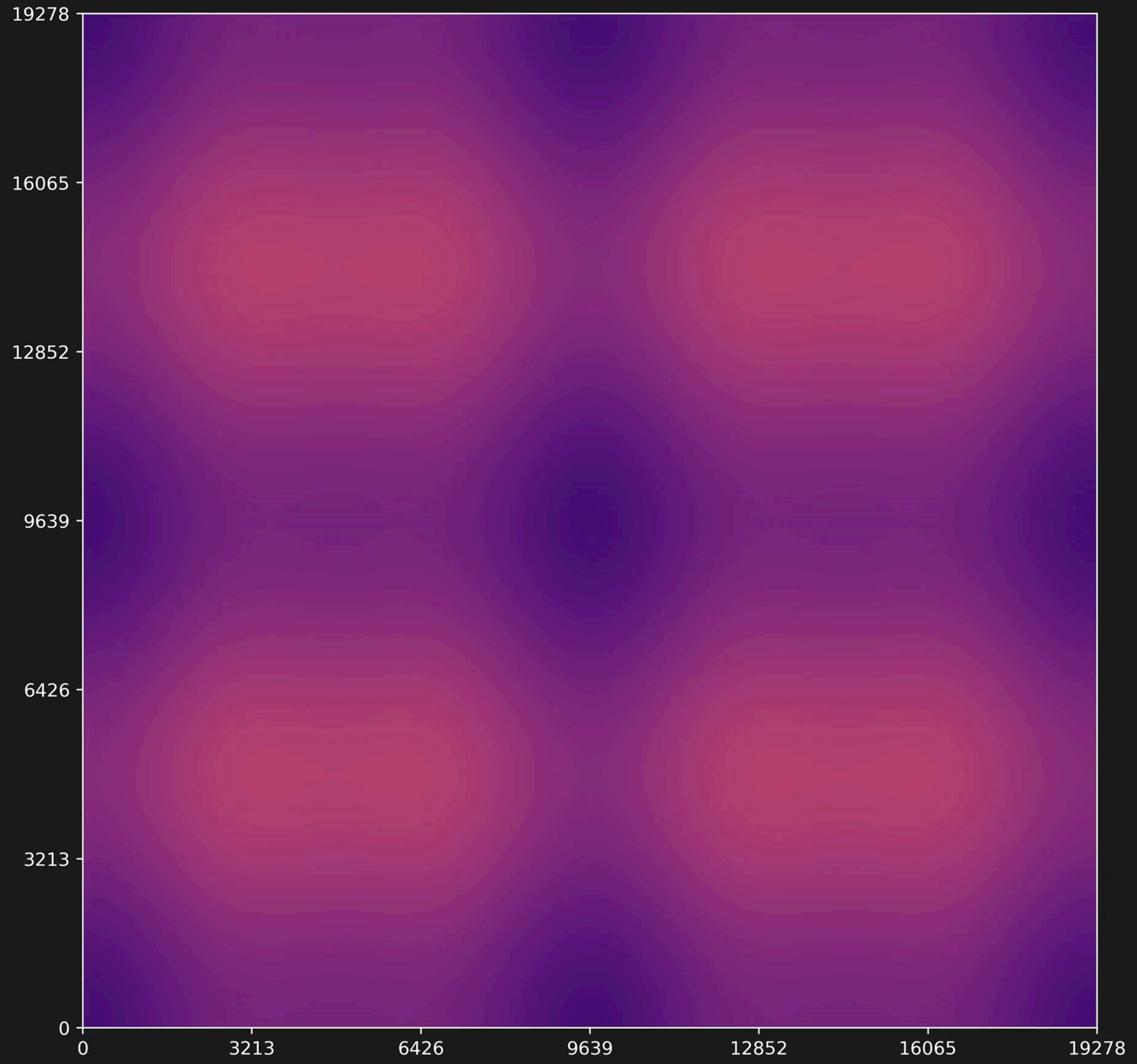
ORSZAG–TANG VORTEX

ENERGY



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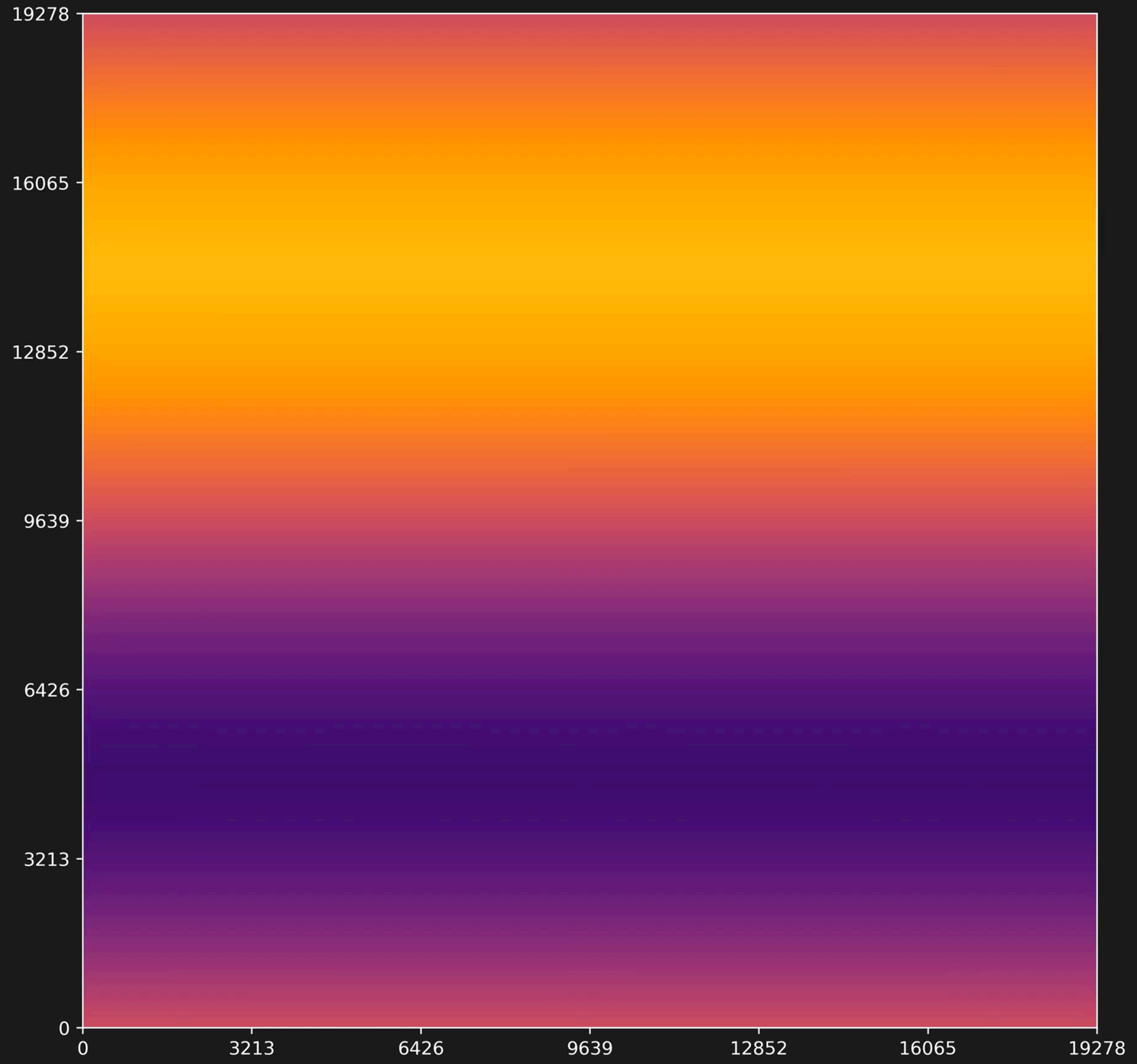
ORSZAG–TANG VORTEX

P_x



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ORSZAG–TANG VORTEX

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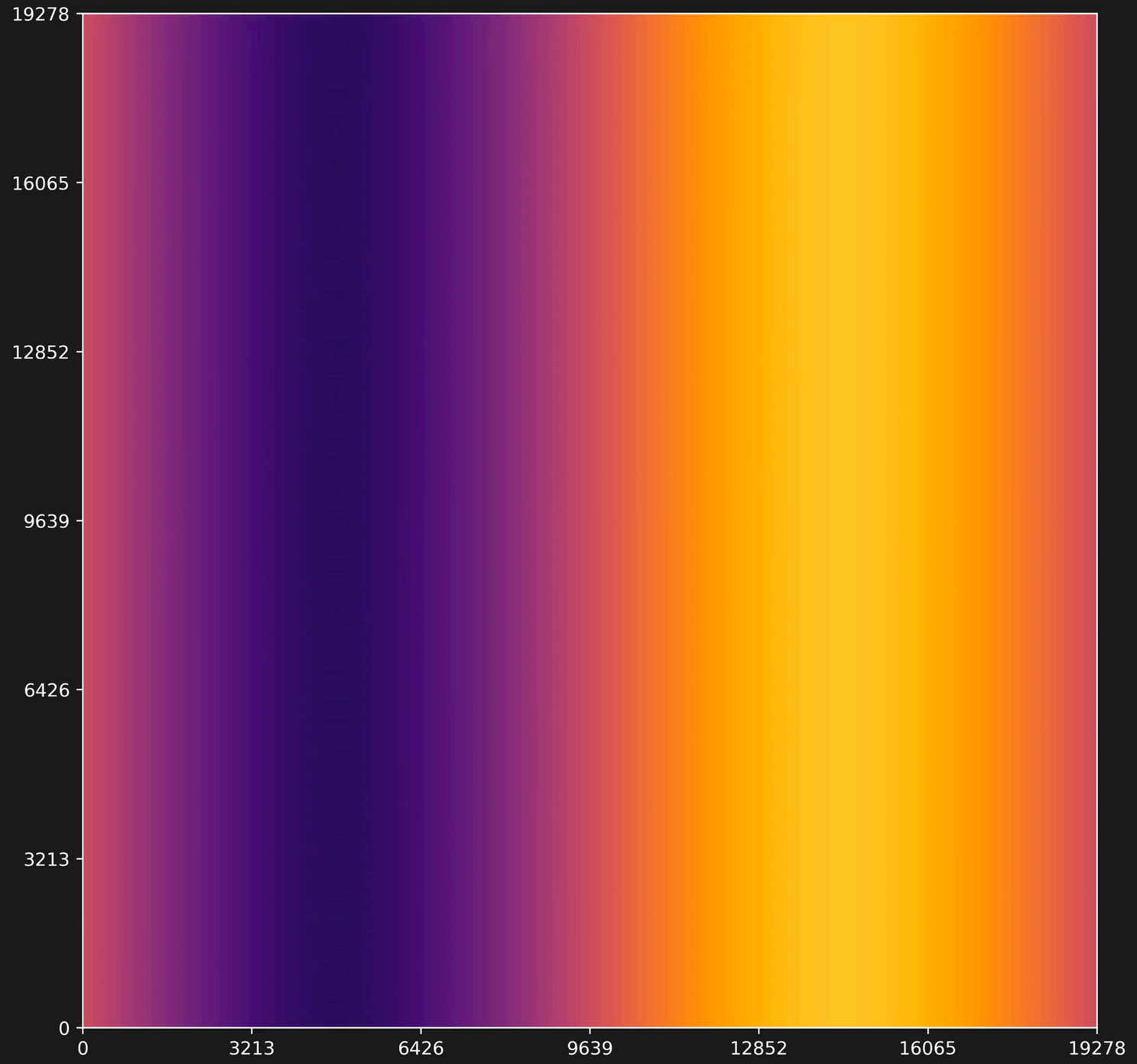

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ORSZAG–TANG VORTEX

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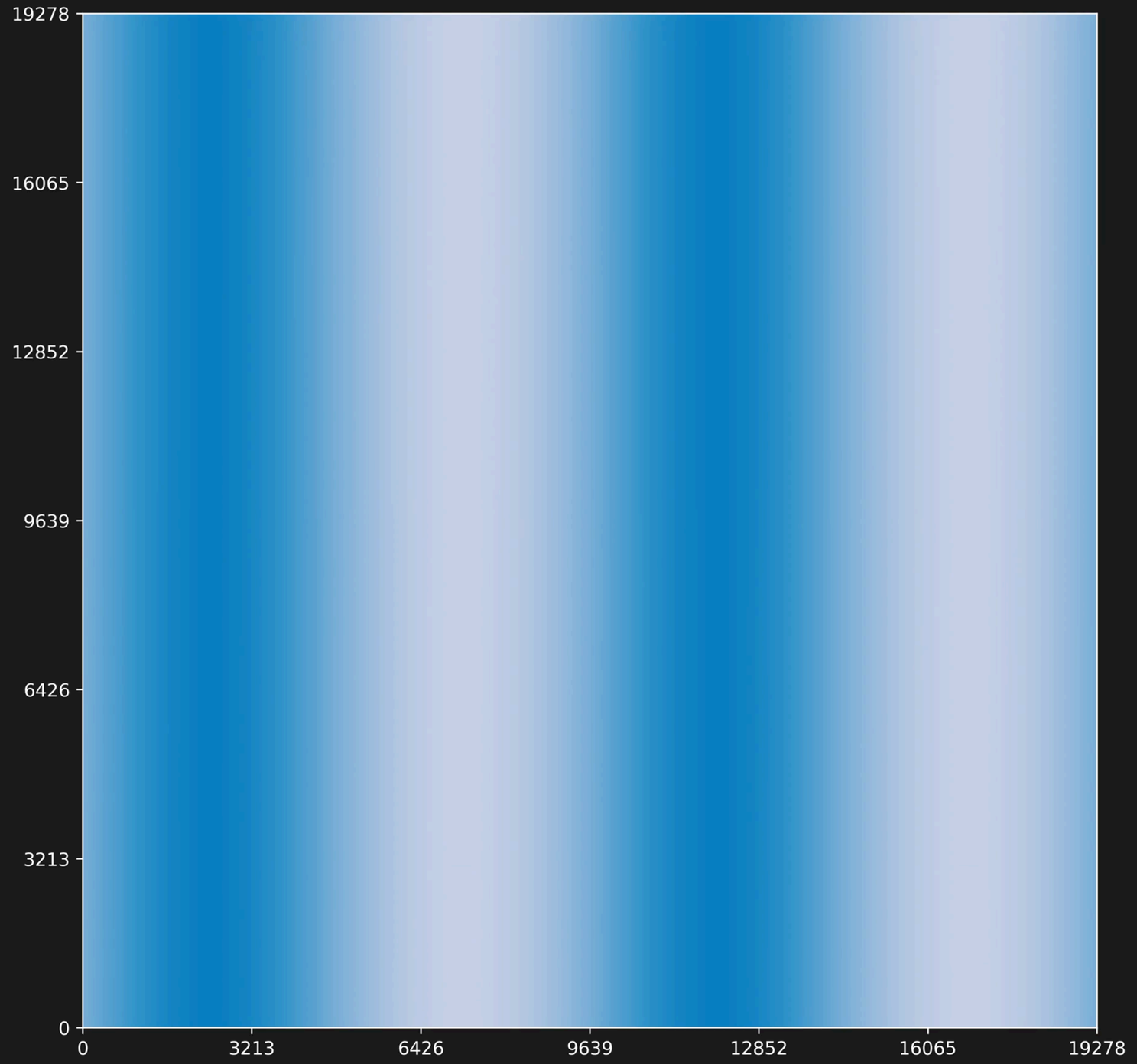

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