DOI:10.5281/zenodo.10120349

State of In Situ Visualization in Simulations: We are fast. But are we inspiring?

EXASCALE COMPUTING PROJECT

In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization (ISAV23)

In conjunction with:
The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC23)

Denver (CO), USA
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LBNL, LLNL, SLAC, CEA, DESY, TAE, CERN

Special thanks to ECP Alpine - Ascent
Cyrus Harrison, Matt Larsen, Nicole Marsaglia et al.

NNSA National Nuclear Security Administration
SciDAC Scientific Discovery through Advanced Computing
U.S. DEPARTMENT OF ENERGY | Office of Science

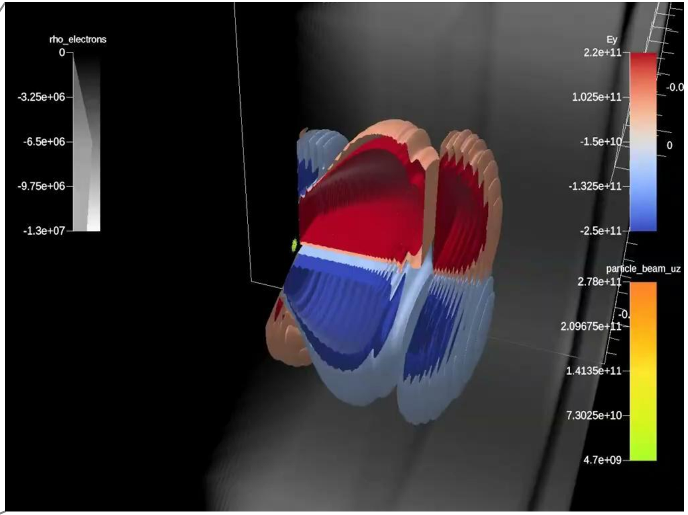
State of In Situ Visualization in Simulations

- **We are fast.** *Scalable Simulations 🤝 Visualization*
  - Our Domain Science
  - Scalable In Situ Analysis & Visualization

- **But are we inspiring?** *Exciting, unsolved challenges*
  - quality: expectations
  - workflows: inputs, animations
  - asynchronous algorithms: stitched, spatially-sliced data

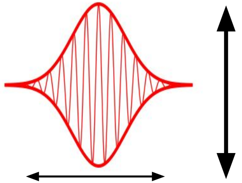
Kinetic Modeling Ecosystem

- Laser-Plasma, Accelerators & Beams
- 4+ Multi-GPU Codes, Libraries, Standards
- **WarpX**: 3D Time-Integrated PIC Code



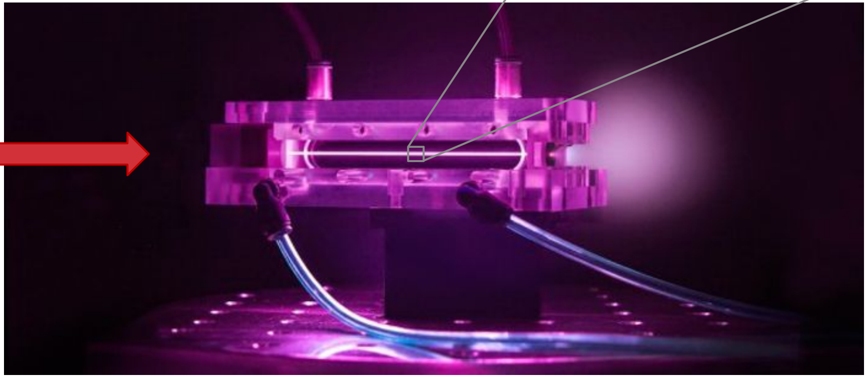
Staging of Laser-Wake-field Accelerators for Next-Gen Colliders

10^{14}W to 10^{16}W



τ=30fs

high power laser pulse

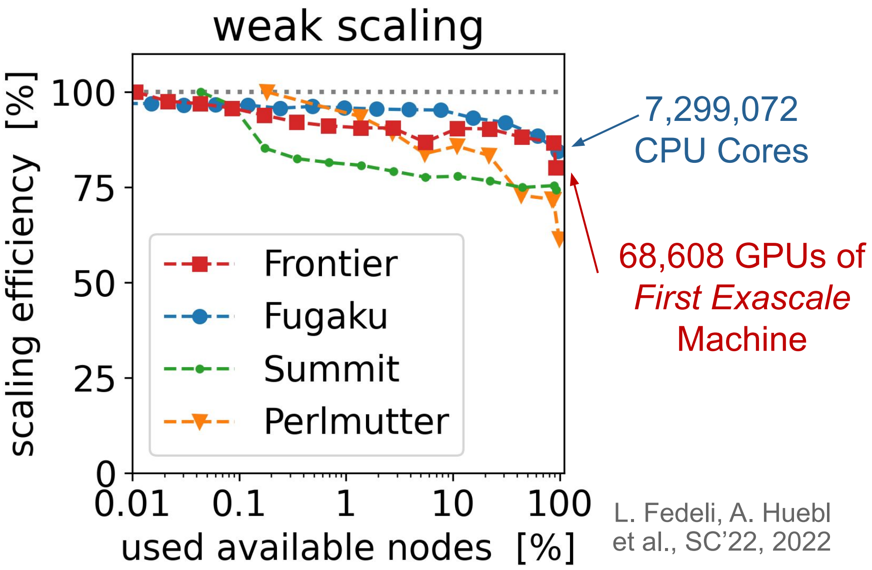


WarpX on 552 Frontier Nodes (4,416 GPUs/GCDs): transv. electric field in an LPA - *Ascent & VTK-m*
N Marsaglia, M Larsen, C Harrison, A Huebl, J-L Vay DOI:10.5281/zenodo.8226853

Plasma	←**Conventional**
100 GV / m	←20 MV/m

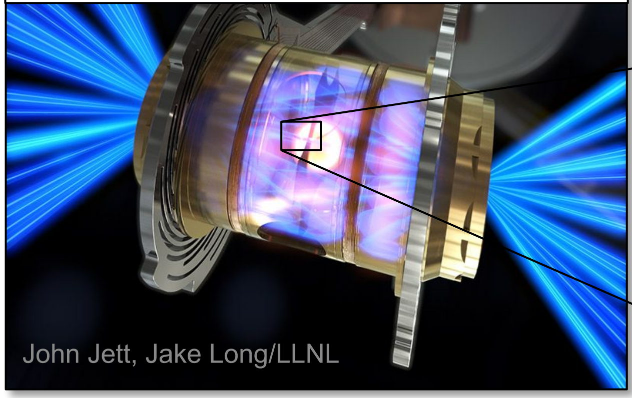
Kinetic Modeling Ecosystem

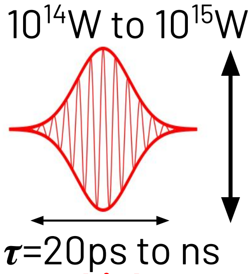
- Laser-Plasma, Accelerators & Beams
- **WarpX:** 2022 ACM Gordon Bell Prize



L. Fedeli, A. Huebl et al., SC'22, 2022

Kinetic effects in Inertial Confinement Fusion

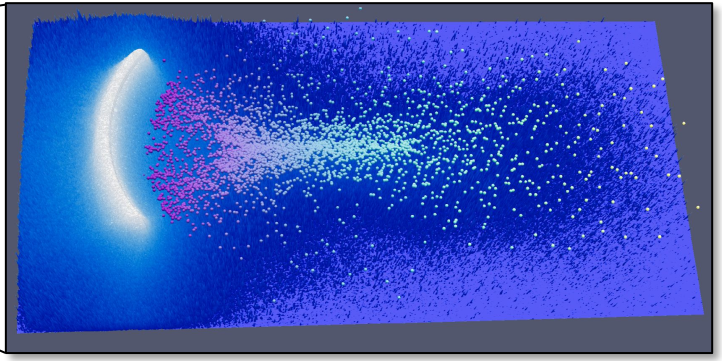




many high power laser pulses

WarpX on Frontier - *ParaView*

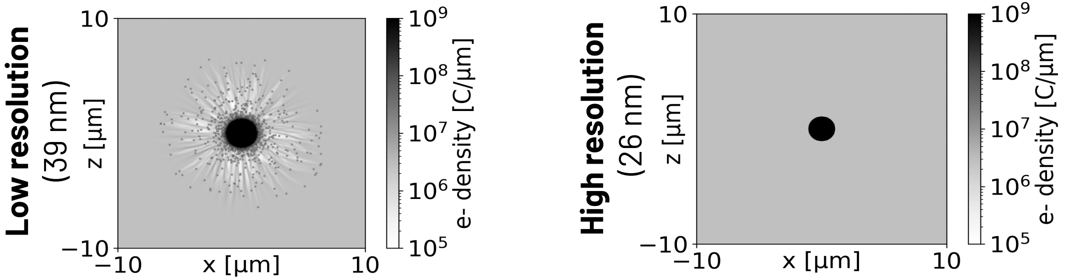
A Huebl, M Garten, J-L Vay, J Ludwig, S Wilks, A Kemp



Through Visualization, we want to Stimulate & Develop Insight

Selected *visual* questions we want to address *in situ*

- **Physics:** Which effects of scale & dimensionality are overlooked in lower fidelity?
- **Dynamics:** Is a (costly) simulation evolving as anticipated?
- **Analytics:** What is the response on a (virtual) detector?
- **Correctness:** Are numerical options and resolution sufficient & stable?



L. Fedeli, A. Huebl et al., SC'22, 2022

  - Are any hardware or software issues/bugs appearing at scale?

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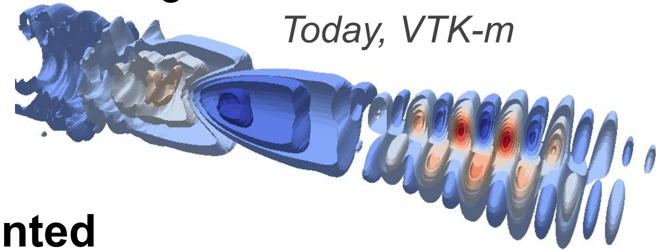
Opportunity 1: Stimulate Insight, Inspire Ideas

Quality of In Situ Generated Vis

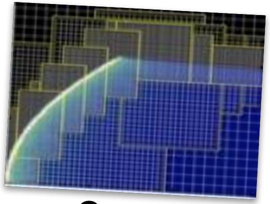
2005
OpenDX

- **Expectations** from traditional vis
  - movies, games, advertising
  - stimulate minds, inspire awe

Today, VTK-m



- **Scalable Methods Wanted**
  - casting soft+hard shadows, tracing reflections, semi-transparent iso-contours, smoothing, volume-rendering >1 overlapping source
    - sorting collisions with objects, etc.
    - notoriously non-local and are thus challenging for multi-GPU



What we willing to trade for this?
Add/exploit artificial locality from refinement, reduction, occlusion/defocus/fog, …?

Opportunity 2: User-Facing Workflows

Usage could be easier

- New tool = New input
    - standardize visualization scenes[1]
    - rapid scene design
- exchange scenes: post-processing GUIs ⇆ in situ
    - ambience: load external/STL geometries

[1] Conduit, OpenUSD.org, ANARI

```yaml
-
  action: add_pipelines
  pipelines:
    contour_pipeline:
      f0:
        params:
          field: Ey
          levels: 16
        type: contour
-
  action: add_scenes
  scenes:
    ey_contour_pc:
      plots:
        p0:
          field: Ey
          pipeline: contour_pipeline
          type: pseudocolor
      renders:
        r1:
          camera:
            azimuth: 90.0
          image_prefix: "ey_contour_pc_"
    ey_volrend:
      plots:
```

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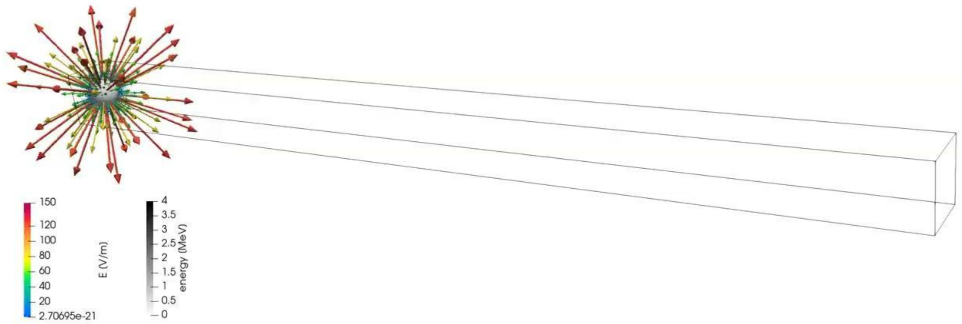

WarpX - *ParaView*
A Formenti

- **Animations**
  - flicker: iso-contours, glyphs, streamlines
  - reason: roughness of simulation data and steps selected
  - challenge: smooth transitions/animations as in web/CSS?

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Opportunity 3: Visualize Partial Data - Stitch it Over Time

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

Often, we cannot yet in situ visualize the *right* data.

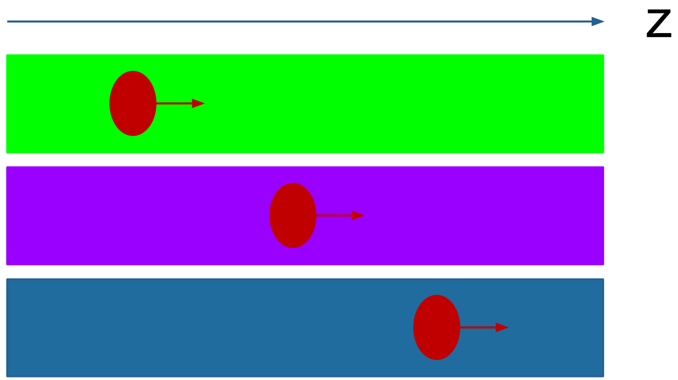
- Traditional, time-based iteration
  - every cell & particle are modeled at the same time t
  - $t_{n+1} = t_n + \Delta t$

Traditional Domain Decomposition

$t_1 = t_0 + \Delta t$

$t_2 = t_1 + \Delta t$

$t_3 = t_2 + \Delta t$



sort-last parallel render

sort-last parallel render

sort-last parallel render

K Moreland and B Wylie, IEEE PVG (2001)   K Moreland et al., SC11 (2011)
https://www.kennethmoreland.com/scalable-rendering

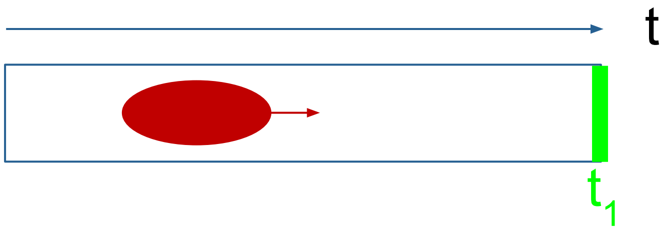
EXASCALE COMPUTING PROJECT

Opportunity 3: Visualize Partial Data - Stitch it Over Time

Often, we cannot yet in situ visualize the *right* data.

- Codes in BLAST: WarpX w/ boosted frame, HiPACE++, ImpactX
- domain-decomposition: space (2D) + time (1D)
- render streamed, spatially-sliced data

Optimal Ref. Frame for Compute



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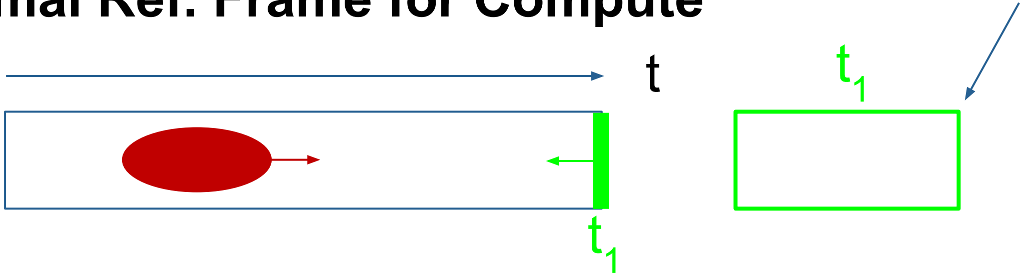
back-transformed data



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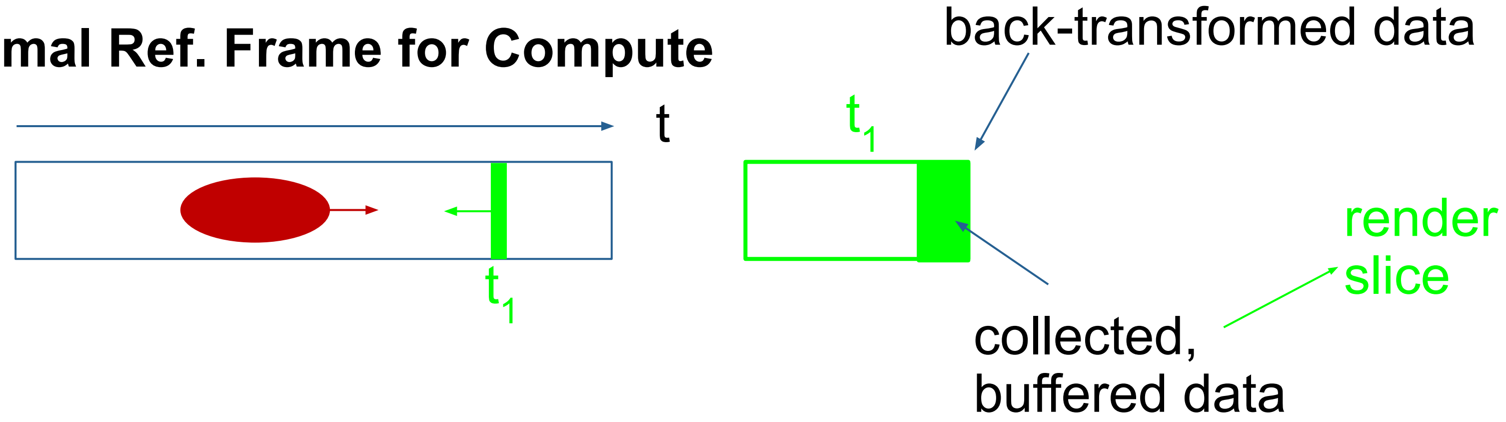

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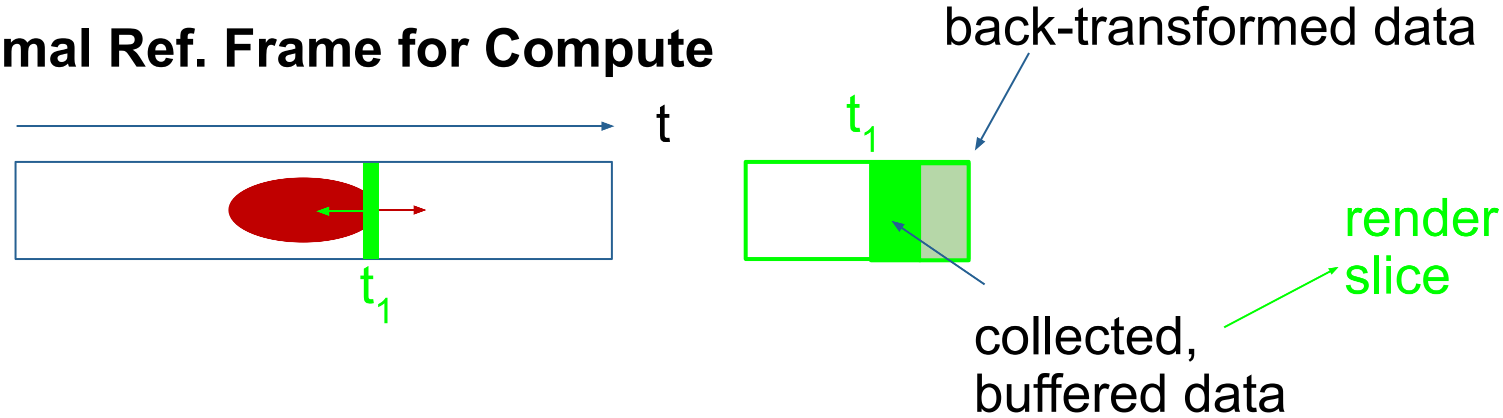

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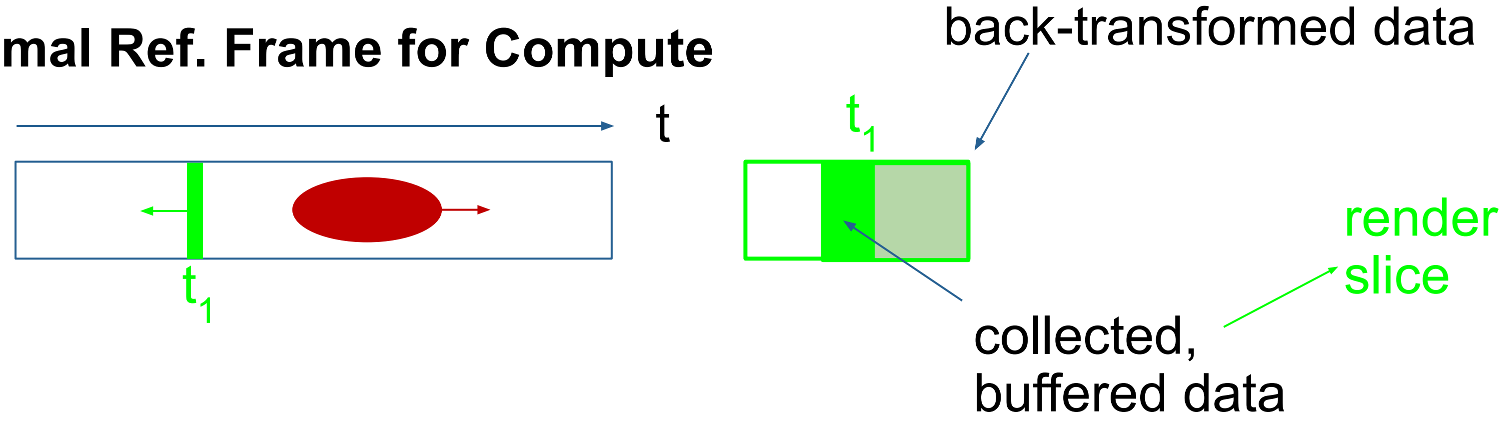

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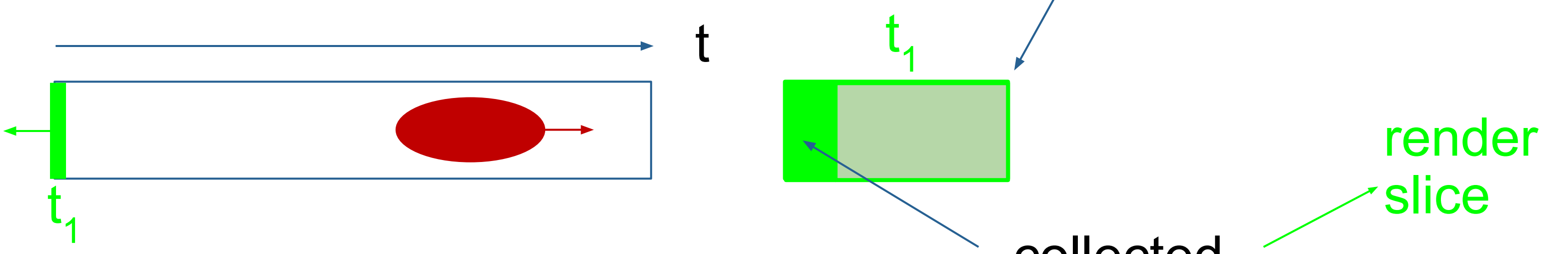

Now: *sort-last parallel* ***composition*** of **all rendered slices** for t_1 .

State-of-the-art: Fallback to slice-wise, full data <u>output</u> - vis. in post!

Opportunity 3: Visualize Partial Data - Stitch it Over Time

BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

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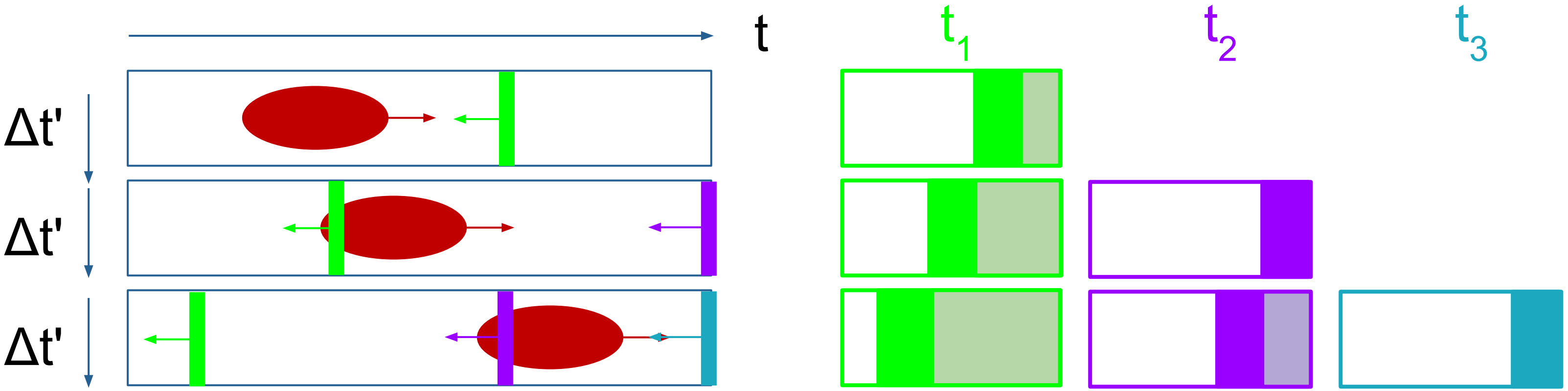

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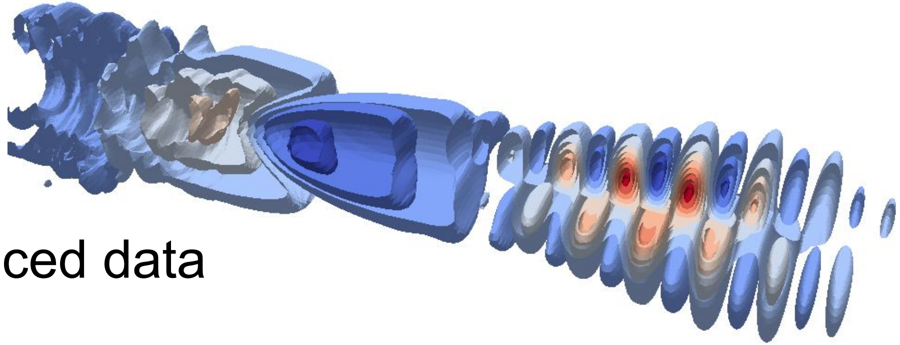
Thank you for your Attention - Let's Address those Opportunities Together

Opportunity Recap

1) **quality**: expectations
2) **workflows**: inputs, animations
3) **algorithms**: stitched, spatially-sliced data



WarpX: longitudinal electric field in a laser-plasma accelerator
rendered with Ascent & VTK-m

github.com/**ECP-WarpX**
github.com/**openPMD**
github.com/**AMReX-Codes**
github.com/**picmi-standard**

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