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Modeling pre-Exascale AMR Parallel I/O Workloads via Proxy Applications

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- Introduction: AMR outputs and characterization
- Understanding AMReX Castro parallel outputs
- Proxy App: MACSio modeling formulation and results
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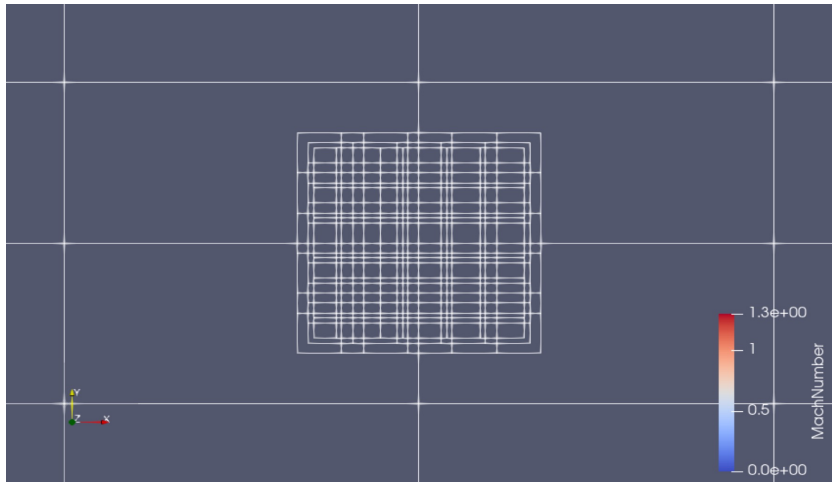
Introduction: AMR outputs

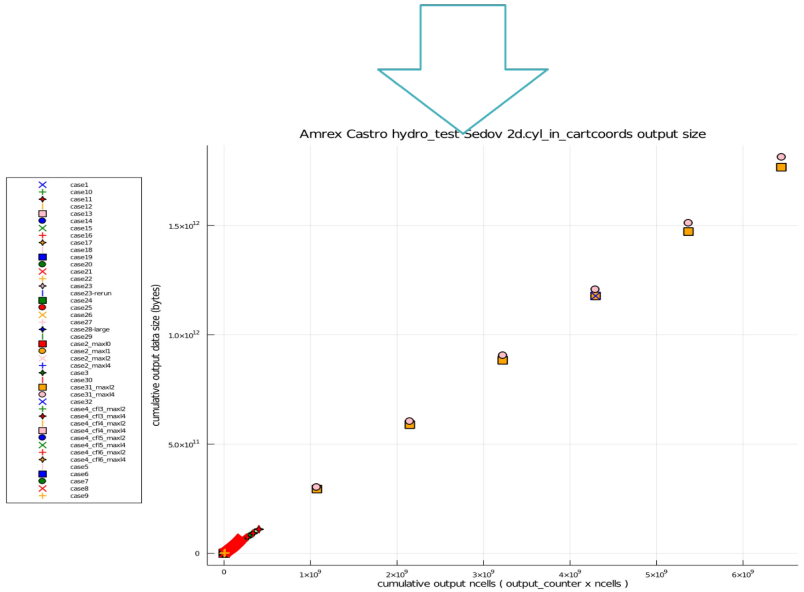
- Adaptive Mesh Refinement (AMR) is a powerful technique for solving partial differential equations (PDEs)
- Depending on user needs, it can cross between compute to I/O bound intensive simulations
- I/O patterns depend on several variables in the meshing, solution, partitioning
- I/O is becoming a bigger bottleneck as we enter the exascale era

Introduction: AMR IO Characterization

- **Understanding I/O characteristics of Adaptive Mesh Refinement (AMR) Input/Output Patterns**
- **“Predictability” in pre-Exascale systems (Summit) via proxy applications.**
- **Cost of Analysis Data and Checkpoint-Restart**
- **Better decision making for AMR codes**
  - **When do I use Burst Buffers or the File System?**
  - **How often do I write data? Checkpoint? Analysis?**
  - **What’s the I/O cost overhead in my application?**
  - **How much “in situ” data can I process?**
  - **What format or backend should I use?**

GOAL: “Develop adaptable modeling and proxy applications frameworks to characterize AMR code I/O for better decision making in the upcoming Exascale era”





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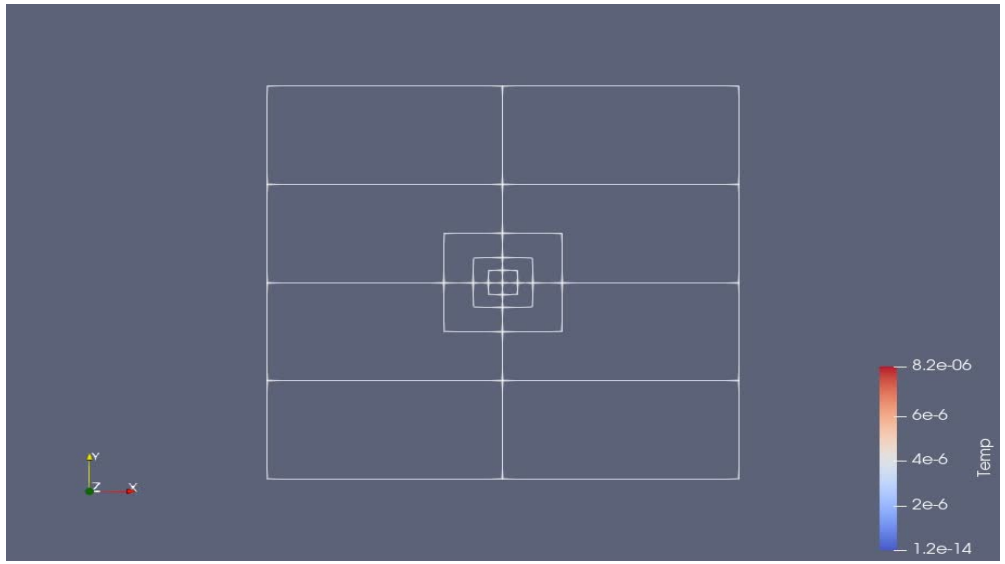
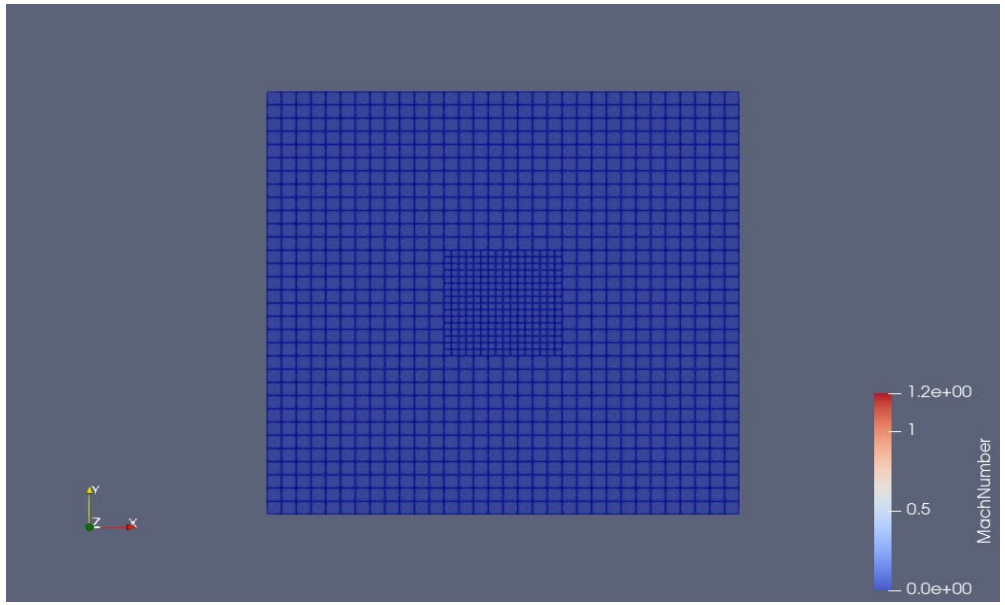
Understanding AMReX Castro parallel outputs

- **Output production rate depends on**
  - **physical and simulation parameters**
  - **mesh generation**
  - **parallel partition**
- **Not easily predictable**
- **Let's look at a simple Sedov hydrodynamic test**
- **Symmetric, 2D Mach number using 3 levels**





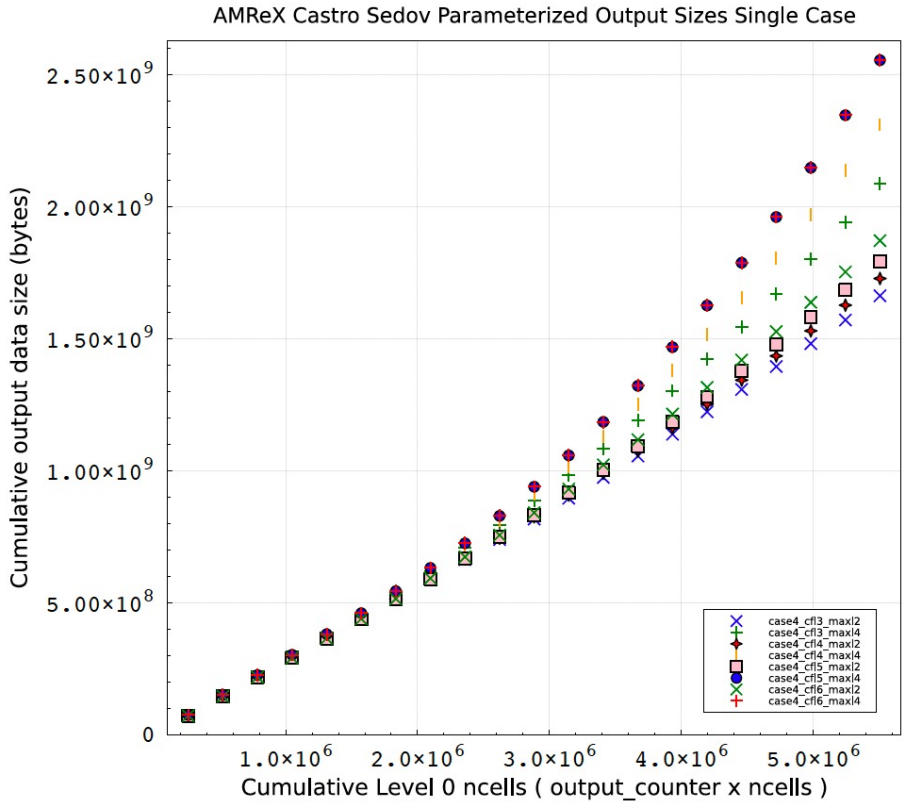
Understanding AMReX Castro parallel outputs

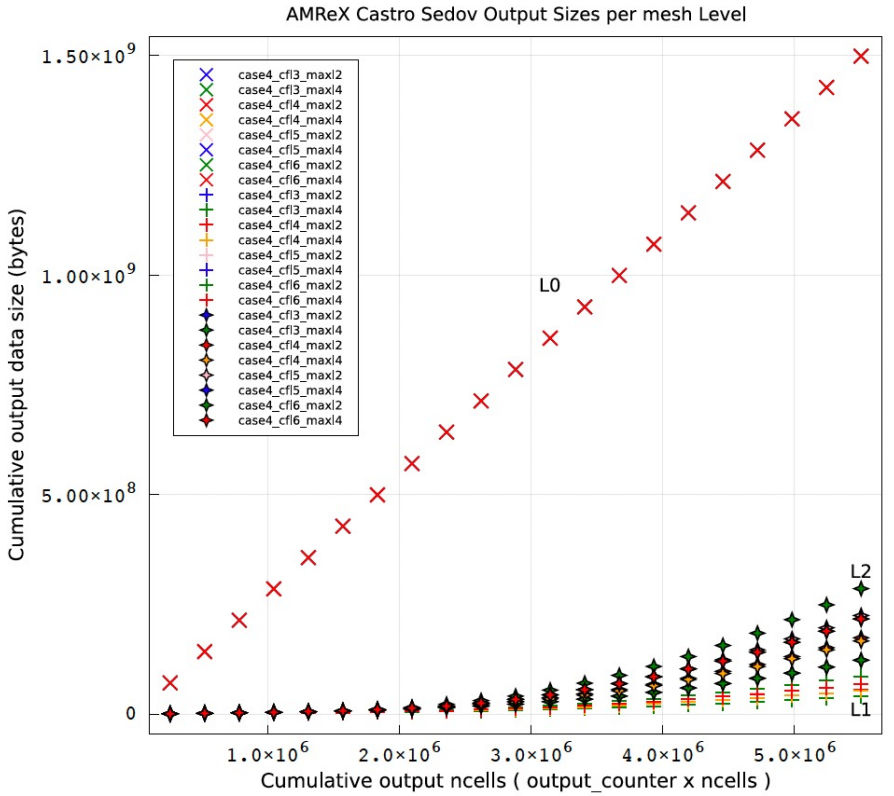
- **AMReX Castro https://amrex-astro.github.io/Castro/ produces analysis data on a <Timestep, Level, Rank> basis**

```
AMReX Castro Simulation Output
├── sedov_2d_cyl_in_cart_plt00000 (step directory - one per plot interval)
│   ├── Header
│   ├── job_info
│   ├── Level_0 (level directory - one per level)
│   │   ├── Cell_D_00000 (cell data file - one per rank)
│   │   ├── Cell_D_00001
│   │   ├── ...
│   │   ├── Cell_D_0000N (N = number of MPI processes)
│   │   └── Cell_H (mesh metadata file)
│   ├── Level_1
│   ├── Level_2
│   ├── ..
│   └── Level_L
├── sedov_2d_cyl_in_cart_plt00020
├── ..
└── sedov_2d_cyl_in_cart_pltMMMMM (final step output)
```

Understanding AMReX Castro parallel outputs

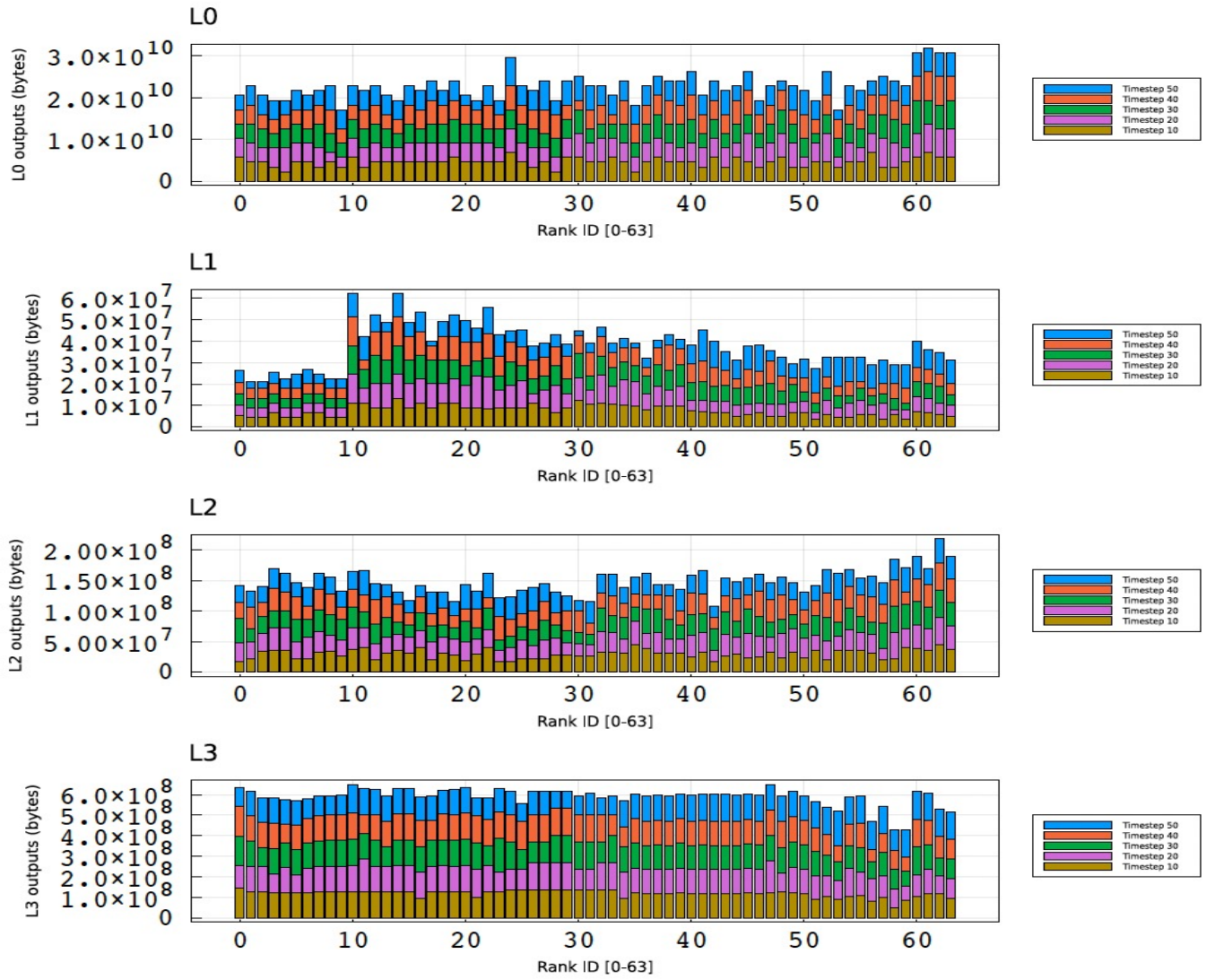
- **<Timestep, Level> → "smooth production"**
- **<Rank> → "unpredictable production"**





Understanding AMReX Castro parallel outputs

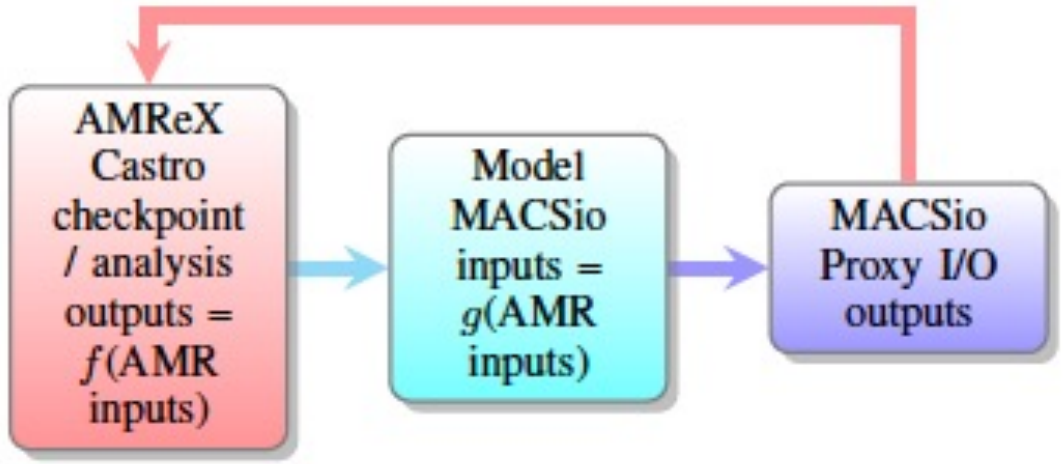
- **<Rank> → "unpredictable production"**



Proxy App: MACSio modeling formulation

- Generate cases on Summit, AMReX Castro to do a characterization study. [Outputs] = f([Inputs])
  - Inputs: problem size, output frequency, partition, **AMR levels, CFL condition**
  - Outputs: analysis data sizes
- MACSio https://github.com/LLNL/MACSio is a simple MPI based executable that produces "Kernel" outputs via arguments. <Step, Rank> production

```
$ mpirun -np 32 macsio --interface  default --avg_num_parts 8 --part_size 100K --parallel_file_mode MIF 32
```




```
MACSio data output
├─ data
│  └─ macsio_json_{taskID}_{stepID}.json
│     ├─ macsio_json_00000_000.json
│     ├─ macsio_json_00000_001.json
│     ├─ ...
│     ├─ macsio_json_00000_{nsteps}.json
│     ├─ ...
│     └─ macsio_json_{nprocs}_{nsteps}.json
└─ metadata
   └─ macsio_json_root_{stepID}.json
      ├─ macsio_json_root_000.json
      ├─ macsio_json_root_001.json
      ├─ ...
      └─ macsio_json_root_{nsteps}.json
```

Proxy App: MACSio modeling formulation

- Generate cases on Summit, AMReX Castro to do a characterization study. [Outputs] = f([Inputs])
  - Inputs: problem size, output frequency, partition, **AMR levels, CFL condition**
  - **Understand parameters that drive I/O**

Listing 2: Input configuration file for the AMReX-Astro Castro Sedov inputs.2d.cyl_in_cartcoords case.

```
# INPUTS TO MAIN PROGRAM
max_step = 500
stop_time = 0.1

# PROBLEM SIZE & GEOMETRY
geometry.is_periodic =  0 0
geometry.coord_sys   =  0  # 0 => cart
geometry.prob_lo     =  0    0
geometry.prob_hi     =  1    1
amr.n_cell           = 32   32

# BC FLAGS
# 0 = Interior 3 = Symmetry
# 1 = Inflow   4 = SlipWall
# 2 = Outflow  5 = NoSlipWall
castro.lo_bc       =  2   2
castro.hi_bc       =  2   2

# WHICH PHYSICS
castro.do_hydro = 1
castro.do_react = 0

# TIME STEP CONTROL
# CFL number for hyperbolic system
castro.cfl            = 0.5
# scale back initial timestep
castro.init_shrink    = 0.01
# maximum increase in dt
# over successive steps
castro.change_max = 1.1

# DIAGNOSTICS & VERBOSITY
# timesteps between computing mass
castro.sum_interval = 1
```

Parameter	Range
amr.max_step	40 - 1000
amr.n_cell	(32×32) - $(131,072 \times 131,072)$
amr.max_level	2 - 4 (1 to 3 levels)
amr.plot_int	1 - 20
castro.cfl	0.3 - 0.6
nprocs	1 - 1,024
Summit nodes	1 - 512 (1/9 total system)

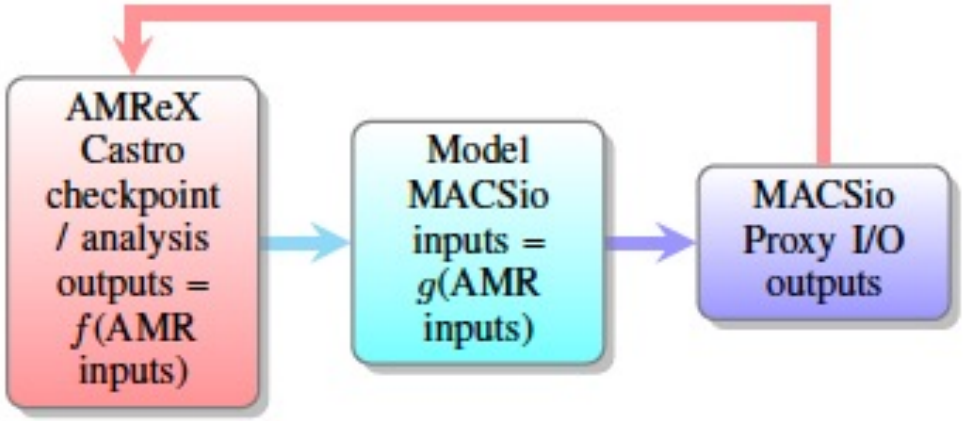
TABLE III: AMReX Castro input configuration file parameters range for the Sedov case running imulations to produce different output sizes.

Proxy App: MACSio modeling formulation

- Relate MACSio inputs to AMReX-Castro inputs

MACSio Argument	Description
`interface`	output type hdf5, json (miftmpl), silo
`parallel_file_mode`	File Mode: multiple independent, single
`num_dumps`	number of dumps to marshal (buffer)
`part_size`	per-task mesh part size
`avg_num_parts`	average number of mesh parts per task
`vars_per_part`	number of mesh variables on each part
`compute_time`	rough time between dumps
`meta_size`	additional metadata size per task
`dataset_growth`	multiplier factor for data growth

TABLE II: MACSio command line arguments used to model AMReX-Castro outputs.



Functional form:

```
jsrun -n nproc
macsio
 --interface miftmpl
 --parallel_file_mode MIF nproc
 --num_dumps amr.max_steps / amr.plot_int
 --part_size f(amr.n_cell)
 --avg_num_parts 1
 --vars_per_part 1
 --compute_time f(platform,all_inputs)
 --meta_size f(all_inputs)
 --dataset_growth f(amr.n_cell,castro.cfl,amr.max_level,...)
```

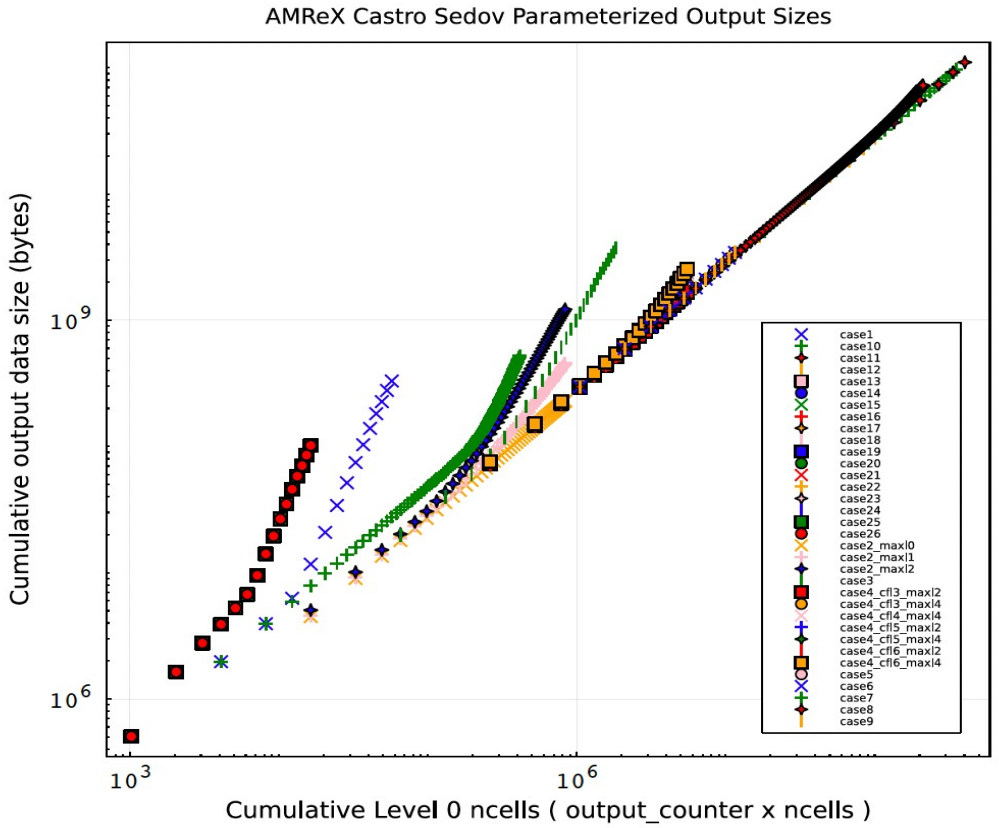
$$\texttt{part\_size} = f\frac{8\,Nx\,Ny}{nprocs}\ [bytes]$$

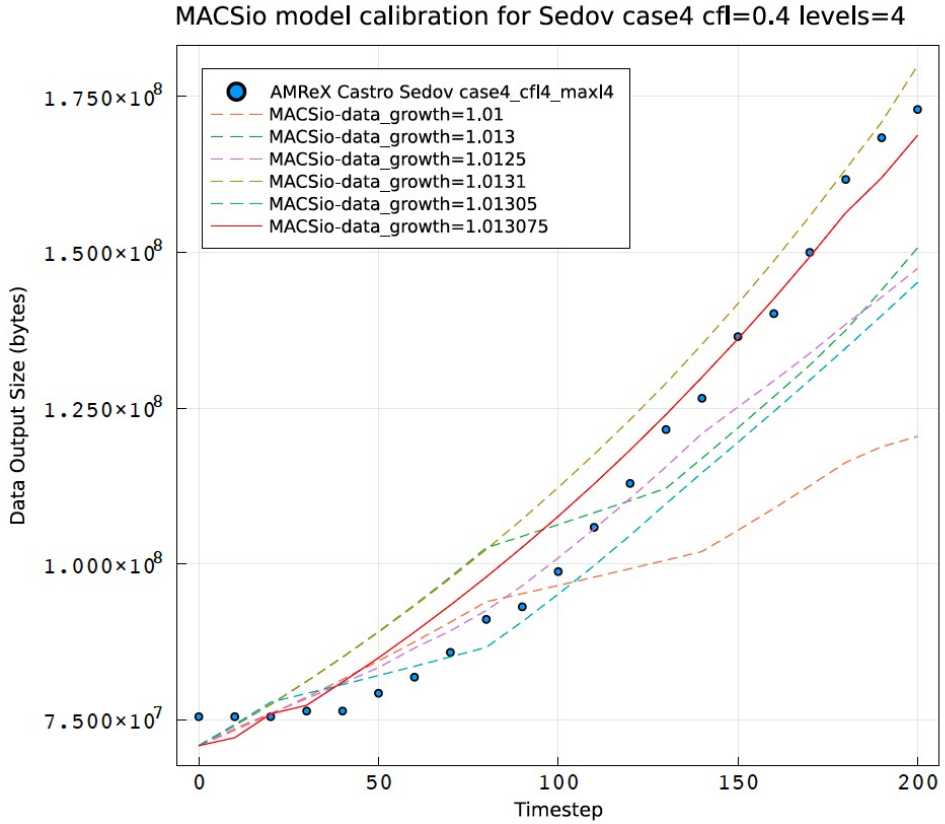
$$f \approx [23 - 25]$$

Proxy App: MACSio modeling results

- Run the AMReX-Castro Sedov baseline case over several configurations on the Summit supercomputer
- Match MACSio model with Sedov output sizes until convergence
- Validate the model over several Sedov configurations

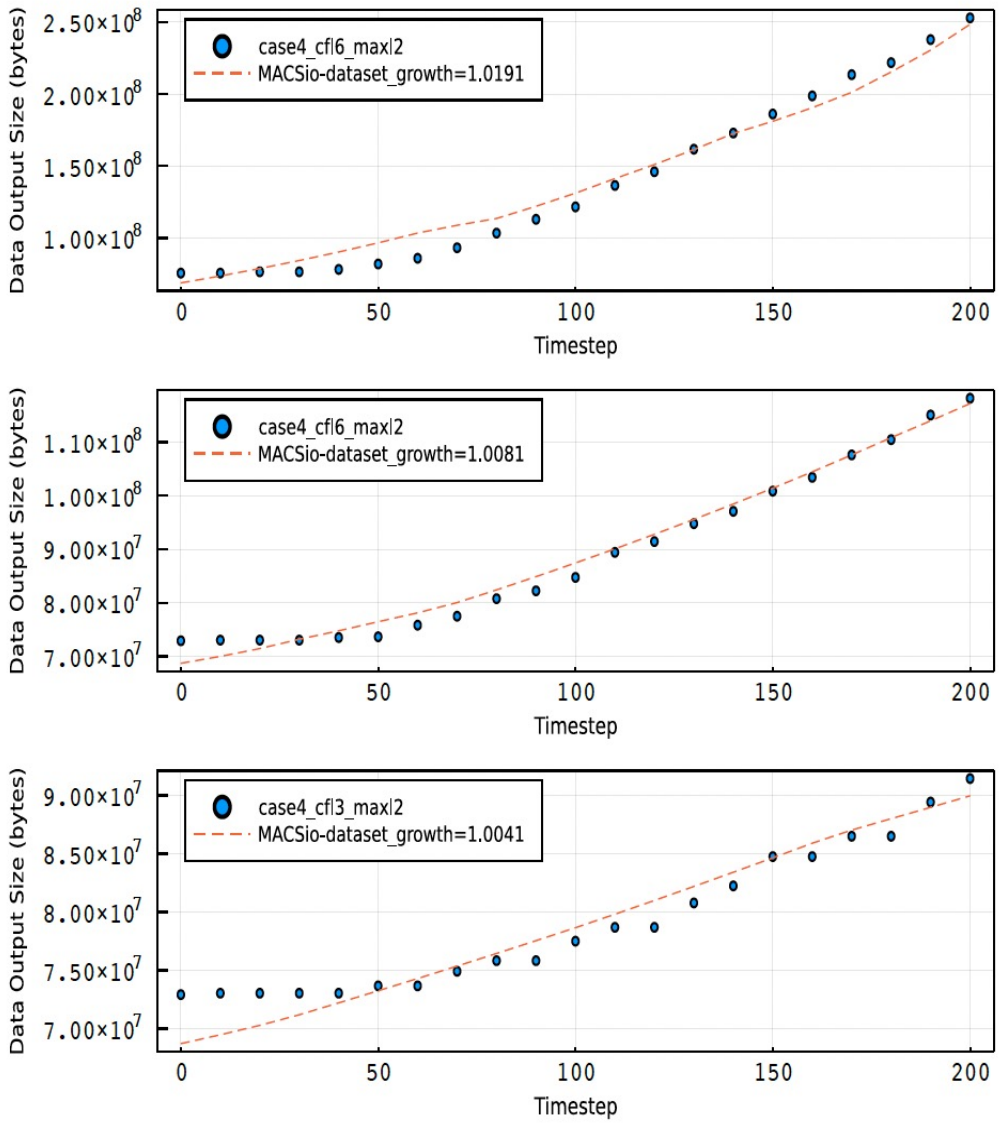
$$\texttt{part\_size} = f\frac{8\,Nx\,Ny}{nprocs}\ [bytes]$$
$$f \approx [23 - 25]$$





Proxy App: MACSio modeling results

- Validate over different cases to model overall "Timestep" output to a certain degree of confidence



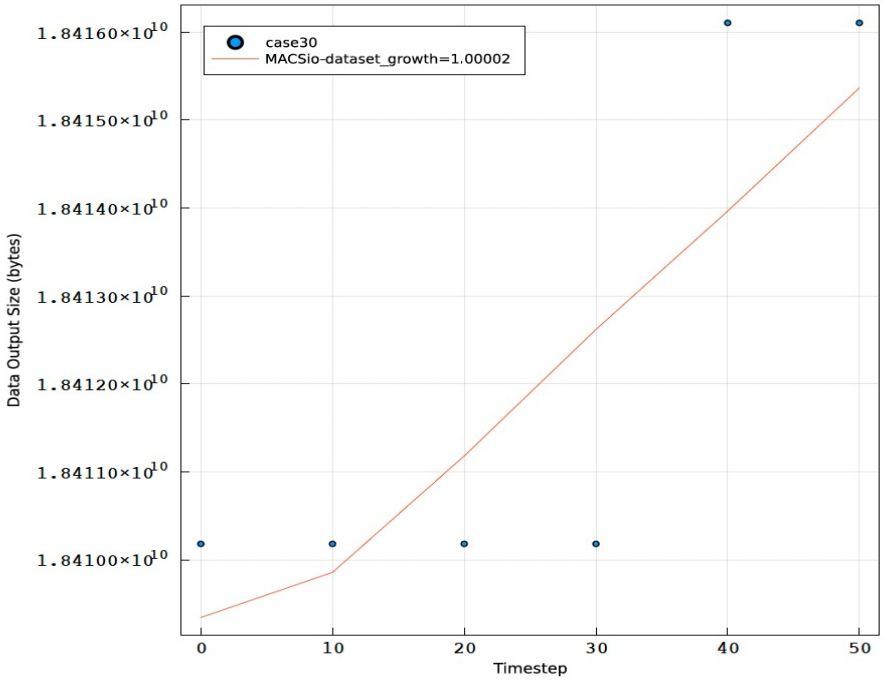


Fig. 11: Comparison of a large L0 mesh $= 8192 \times 8192$ Sedov non-smooth simulation output against the proposed MACSio kernel model.

Summary and Future Work

- We present a simple model formulation for understanding Adaptive Mesh Refinement data outputs via a proxy application like MACSio
- Empirical models can encapsulate the unpredictable per-rank parallel I/O rates up to model AMR levels and timestep data output rates for a range of problem sizes on the Sedov hydrodynamics case
- Future Research Questions:
  - Can we extend this formulation for other AMR configurations?
  - Do we need better granularity in the proxy app and other backends (HDF5, ADIOS2)?
  - Can proxy based modeling help understand exascale AMR I/O bottlenecks?
  - Can we provide autotune system policy for AMR applications at scale?

Acknowledgements

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Thanks!