GPU Accelerated Linear Solvers for Implicit Time Integrators in the SUNDIALS Library

SIAM CSE25, MS9

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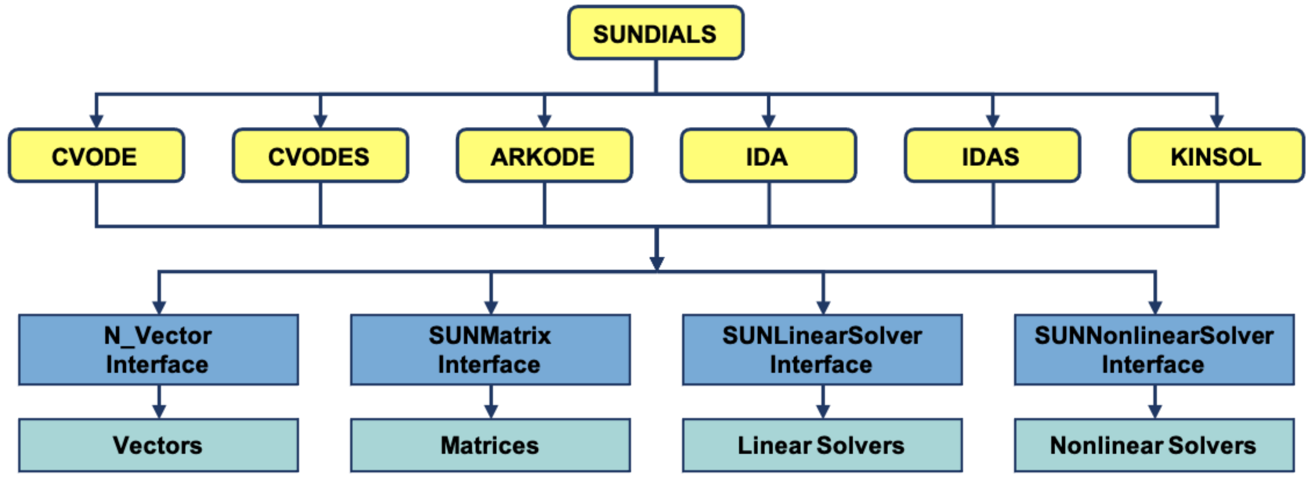
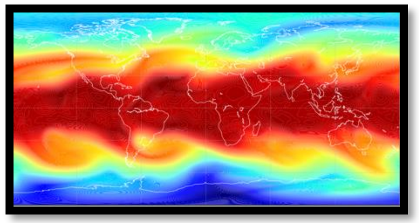
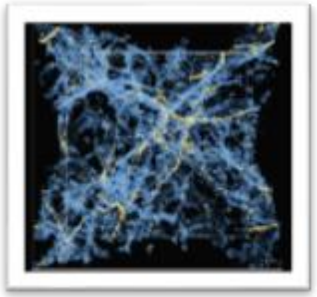
SUNDIALS Overview



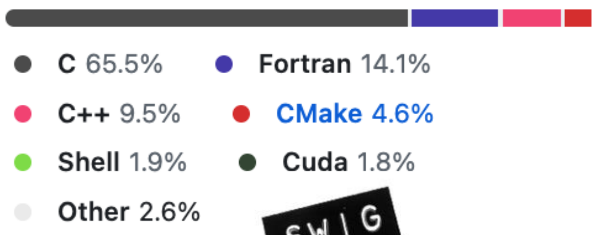
CVODE solves ODEs, $\dot{y} = f(t, y)$, with LMMs, **ARKODE** solves ODEs with one-step methods and supports IMEX + multirate, **IDA** solves DAEs, $F(t, y, \dot{y}) = 0$, **KINSOL** solves nonlinear algebraic systems, **S** variants add sensitivity analysis.


Atmospheric Dynamics


Cosmology

Combustion

Languages:



Continuous Integration with:

Documentation:

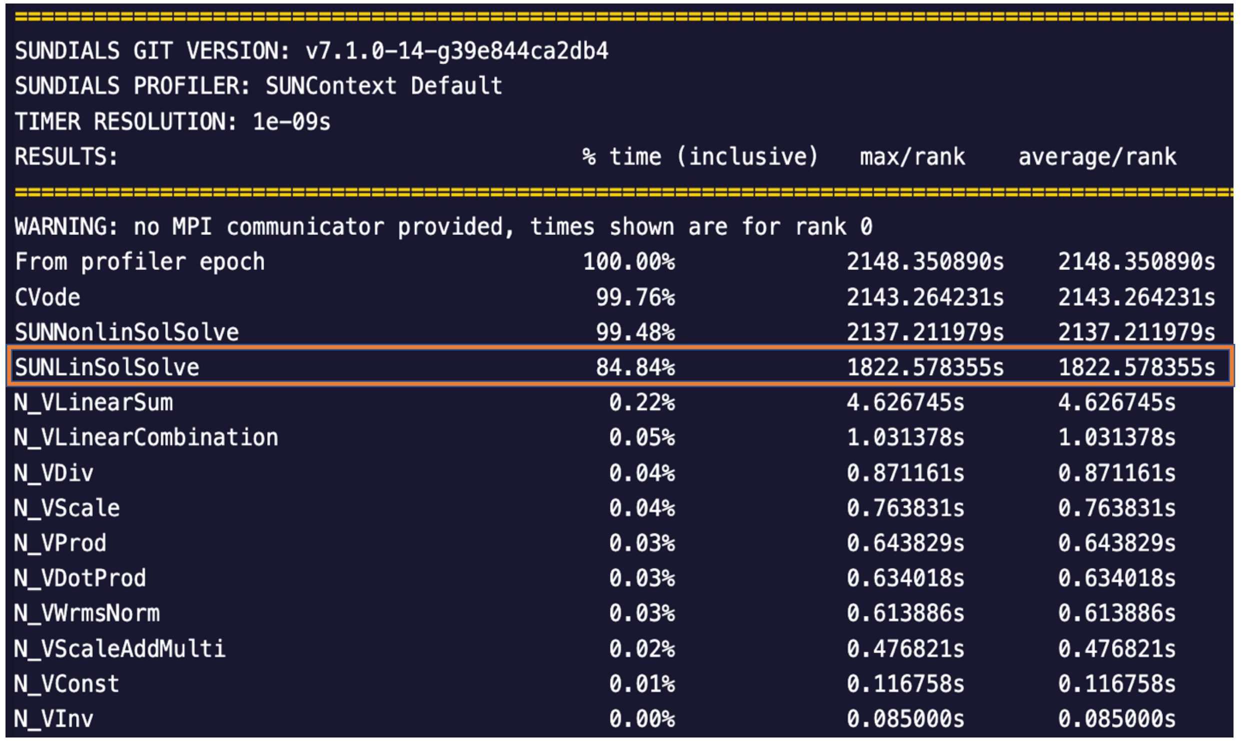
- Optional interfaces to 15 third-party libraries (for solvers and other stuff)!
- Supports NVIDIA, AMD, and Intel GPUs directly and and through RAJA/Kokkos
- Runs on Windows, MacOS, Linux, x86, ARM, Power etc., at a wide range of scales
- Visit computing.llnl.gov/projects/sundials for info

Implicit integrators require efficient linear solvers

- Implicit time integrators are well suited for stiff ODEs, $y'(t) = f(t, y(t))$
- Require us to solve an implicit system iteratively *within every time step*, $F(y^n) = y^n - \gamma f(t_n, y^n) - a_n = 0$
- With modified Newton's method, we must solve a linearized system *within every iteration within every time step*,

$$(I - \gamma J)\delta_{m+1} = -F(y^{n(m)})$$

$$J = \frac{\partial f}{\partial y}, \delta_{m+1} = y^{n(m+1)} - y^{n(m)}$$



```
===========================================================================================
SUNDIALS GIT VERSION: v7.1.0-14-g39e844ca2db4
SUNDIALS PROFILER: SUNContext Default
TIMER RESOLUTION: 1e-09s
RESULTS:                                        % time (inclusive)    max/rank     average/rank
===========================================================================================
WARNING: no MPI communicator provided, times shown are for rank 0
From profiler epoch                              100.00%         2148.350890s    2148.350890s
CVode                                             99.76%         2143.264231s    2143.264231s
SUNNonlinSolSolve                                 99.48%         2137.211979s    2137.211979s
SUNLinSolSolve                                    84.84%         1822.578355s    1822.578355s
N_VLinearSum                                       0.22%            4.626745s       4.626745s
N_VLinearCombination                               0.05%            1.031378s       1.031378s
N_VDiv                                             0.04%            0.871161s       0.871161s
N_VScale                                           0.04%            0.763831s       0.763831s
N_VProd                                            0.03%            0.643829s       0.643829s
N_VDotProd                                         0.03%            0.634018s       0.634018s
N_VWrmsNorm                                        0.03%            0.613886s       0.613886s
N_VScaleAddMulti                                   0.02%            0.476821s       0.476821s
N_VConst                                           0.01%            0.116758s       0.116758s
N_VInv                                             0.00%            0.085000s       0.085000s
```

Execution profile for In Medium Similarity Renormalization Group simulation using implicit method in SUNDIALS CVODE.

SUNDIALS integrators have time step adaptivity

- Based on the method, estimate the time step error

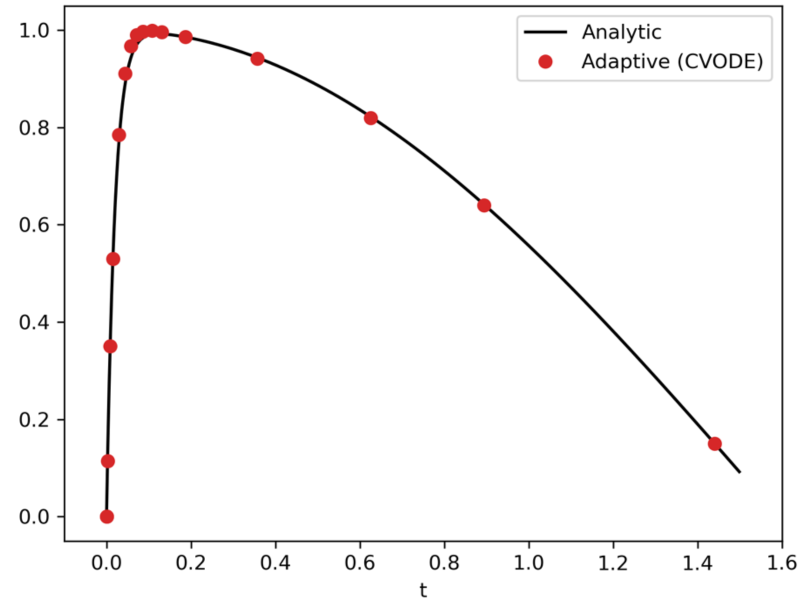
$$\Delta_n \equiv y^{n(m)} - y^{n(0)}$$

  - Accept step if $||\Delta_n||_{WRMS} \leq \epsilon$; Reject it otherwise

$$\|y\|_{\text{wrms}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(w_i\ y_i)^2} \qquad w_i = \frac{1}{RTOL|y_i| + ATOL_i}$$

  - Choose next step, so that $||y^n - y^{n(0)}||_{WRMS}$ should be small

- ARKODE supplies advanced “error controllers” to adapt these step sizes while also meeting other objectives:
  - minimize failed steps
  - maximize step sizes
  - maintain smooth transitions in the step sizes



Adaptivity can give much more efficient (and accurate) results

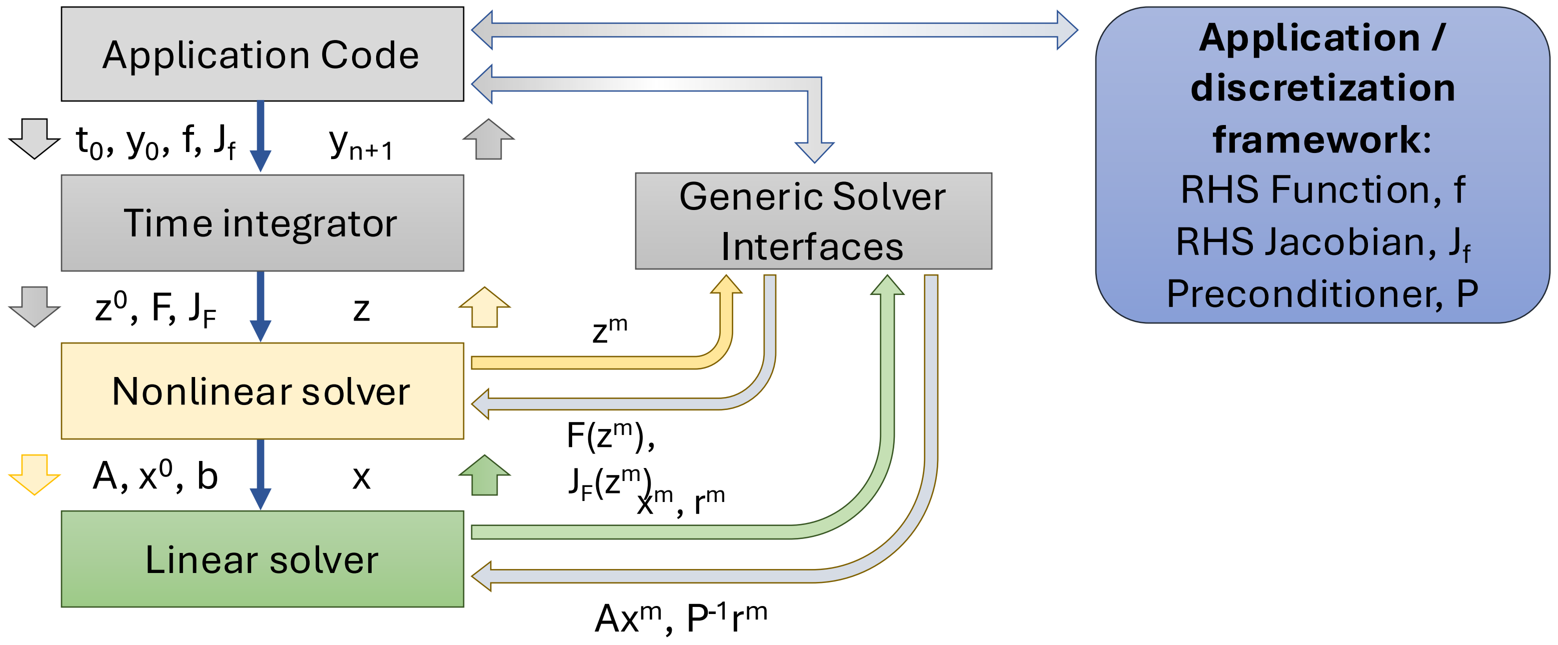
Integrator tolerances propagate down to solvers to keep the error that propagates up small

- Overall goal: keep the nonlinear iteration error from interfering with the local error control
- Stopping criteria for the nonlinear solver: $R||\delta_m||_{WRMS} \leq 0.1\epsilon$,
- The stopping criteria for iterative linear solvers:

$$||(I - \gamma J)\delta_m + F\left(y^{n(m)}\right)||_{WRMS} < 0.05\ (0.1\epsilon)$$

- When iterative linear solver libraries only allow 2-norm*, we must ”translate” our stopping criteria into a 2-norm tolerance
  - It would be great if we could provide solvers our norm

SUNDIALS keeps state data on the GPU



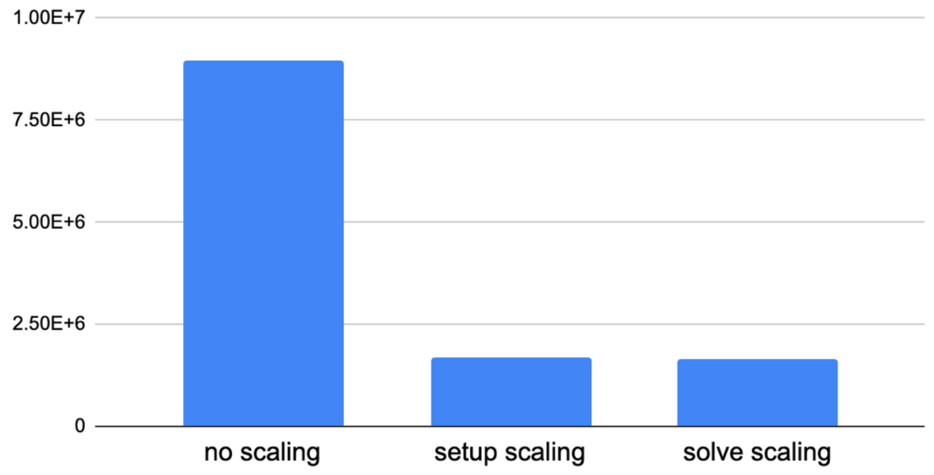
- Integrator logic runs on the CPU, but state data is on the GPU throughout – so solvers receive data on the GPU and should return it to us on the GPU
- We have a memory “helper” API to access application memory pools – solver libraries could benefit from exploiting this too

SUNDIALS iterative “matrix-free” linear solvers

- SUNDIALS has 5 built-in iterative matrix-free linear solvers: CG, BiCGSTAB, GMRES, FGMRES, PTFQMR
- All leverage scaling and preconditioning to balance error between solution components and accelerate convergence
$$(S_1 P_1^{-1} A P_2^{-1} S_2^{-1}) S_2 P_2 x = S_1 \; P_1^{-1} b$$
- S_1 and S_2 are diagonal matrices of scaling factors – within our implicit integrators they are equivalent to diag(ATOL)
- Since these iterative methods only require vector operations, they are GPU-enabled the moment you use a GPU N _Vector

We have an interface to Ginkgo for matrix-based iterative solvers

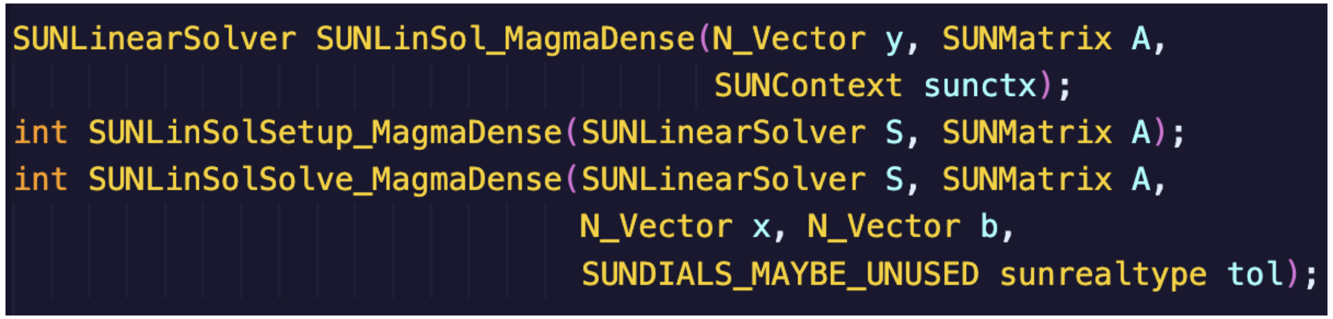
- Our first interface to an iterative solver library
  - Can access most (maybe all) of the iterative solvers in Ginkgo: CG, BiCGSTAB, GMRES, …
  - SUNMatrix implementation uses Ginkgo for matrix storage and operations (sparse or dense)
  - Can use any of Ginkgo's executors (CPU or GPU)
  - Presents as a C++ interface to our users (atypical)
- Issues we encountered resolved by Ginkgo team:
  - Needed matrix operation: $cA + I$
  - Lack of scaling capability hurt performance
  - Couldn't change stopping criteria efficiently



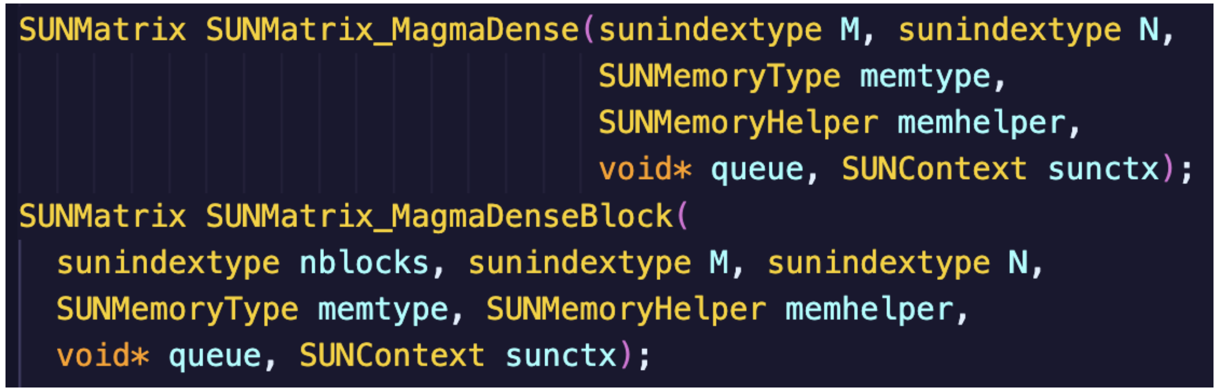
Comparison of Ginkgo batched GMRES in Pele reacting flow problem without scaling (left), with scaling only during matrix setup, and with scaling during every solve. Y axis is the number of linear iterations.

Interface to MAGMA

- We have a unified interface to MAGMA for GPU-enabled dense direct methods for batched and non-batched linear systems
- MAGMA based SUNMatrix and SUNLinearSolver implementations
- Since we lag our Jacobian, we can reuse factorizations across solves
- Call getrf only when Jac. is updated
- Call getrs every nonlinear iteration



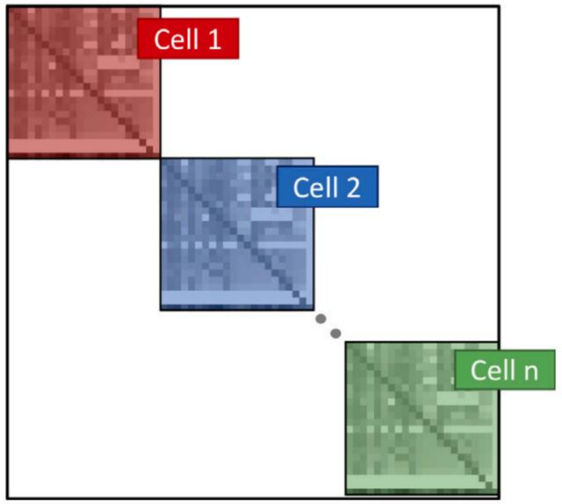
```
SUNLinearSolver SUNLinSol_MagmaDense(N_Vector y, SUNMatrix A,
                                     SUNContext sunctx);
int SUNLinSolSetup_MagmaDense(SUNLinearSolver S, SUNMatrix A);
int SUNLinSolSolve_MagmaDense(SUNLinearSolver S, SUNMatrix A,
                              N_Vector x, N_Vector b,
                              SUNDIALS_MAYBE_UNUSED sunrealtype tol);
```



```
SUNMatrix SUNMatrix_MagmaDense(sunindextype M, sunindextype N,
                               SUNMemoryType memtype,
                               SUNMemoryHelper memhelper,
                               void* queue, SUNContext sunctx);
SUNMatrix SUNMatrix_MagmaDenseBlock(
  sunindextype nblocks, sunindextype M, sunindextype N,
  SUNMemoryType memtype, SUNMemoryHelper memhelper,
  void* queue, SUNContext sunctx);
```

Batched systems arise in reacting flow simulations

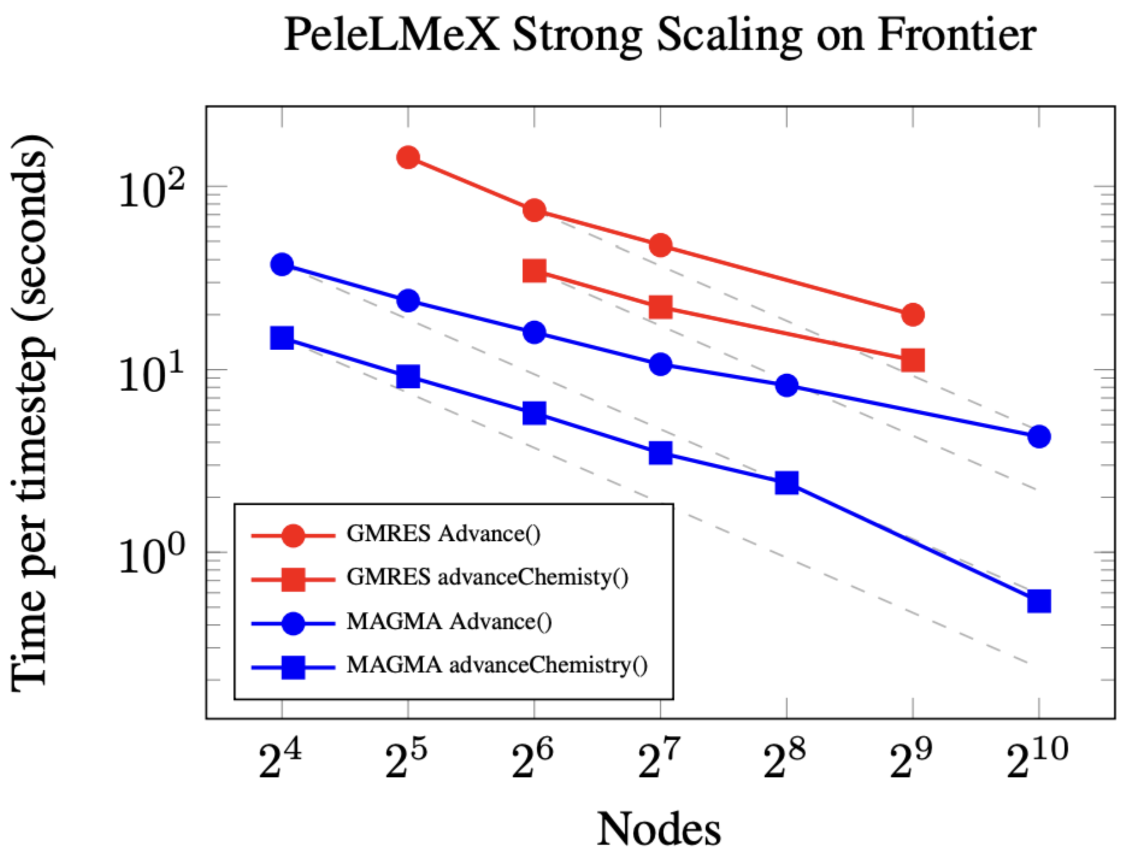
- Pele combustion codes simulate reacting flows, $\frac{\partial u}{\partial t} = F + R$, where R is reaction term
- Operator splitting approach yields independent ODEs for R in each mesh cell
- We batch the ODEs together for integration
  - Increases work for GPU
  - The Jacobian becomes block diagonal
  - Each block has the same sparsity pattern
- Batched linear solvers provide as much as 10x speedup over non-batched in Pele



$$\mathbf{A} = \begin{bmatrix} \mathbf{A_1} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_n} \end{bmatrix}$$

Reacting flow simulation on Frontier with MAGMA

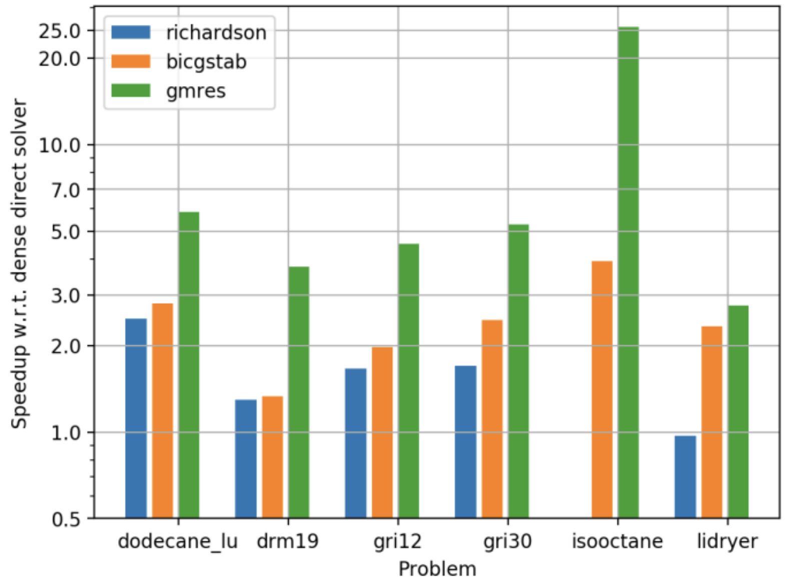
- Lucas Esclapez conducted PeleLMeX simulation strong scaling test on up to 1024 nodes of the Frontier supercomputer
- Compared unpreconditioned, non-batched SUNDIALS GMRES to batched LU in MAGMA
- *advanceChemistry()* routine is the ODE integration



https://doi.org/10.1177/10943420241280060

We worked with Ginkgo on batched iterative solvers

- With our consultation, Ginkgo team developed batched iterative solvers (Richardson, BiCGSTAB, GMRES)
- Data always on the GPU, with 3 total kernel launches (scale, solve, unscale)
- Monolithic solve kernel allows one matrix block per GPU threadblock and allows shared memory to be exploited
- https://doi.org/10.1109/ScalA54577.2021.00010 for details



Problem	Size	Non-zeros (A)	Non-zeros (L+U)
dodecane_lu	54	2,332 (80%)	2,754 (94%)
drm19	22	438 (90%)	442 (91%)
gri12	33	978 (90%)	1,018 (93%)
gri30	54	2,560 (88%)	2,860 (98%)
isooctane	144	6,135 (30%)	20,307 (98%)
lidryer	10	91 (91%)	91 (91%)

Solver performance compared to dense direct batched method from cuSOLVER for different matrices extracted from Pele. Credit Aggarwal et al.

Summary and Conclusions

- Implicit time integrators need efficient linear solvers
- The linear solves are are repeated within a nonlinear iteration within every time step – information can be reused across solves
- Error based time adaptivity affect the solver stopping criteria – would be great if linear solver libraries allowed different norms
- To achieve good GPU performance – solvers must receive the state data on the GPU and give the solution back to us there
- Batched linear solvers allows us to batch ODEs to saturate GPU

computing.llnl.gov/sundials

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Questions?

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