Engagement: Deploying Time Integrators in SciDAC Applications

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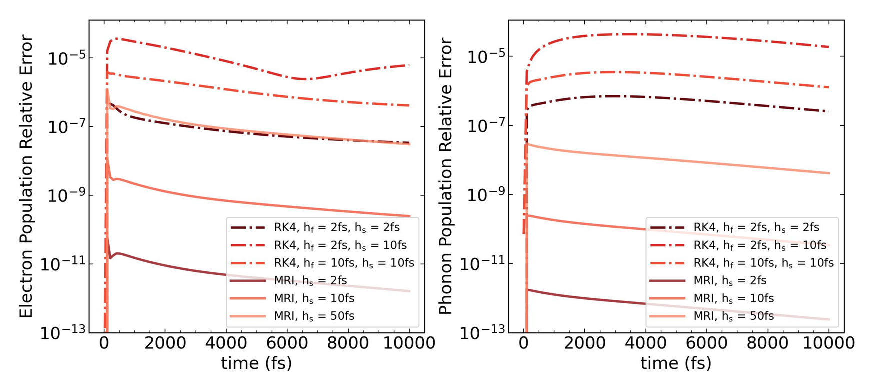
The FASTMath Time Integration team is engaging with several application partnerships across many offices. Technologies being applied include adaptive, ImEx, and multirate integrators as well as support for time evolution using GPUs.

Multirate Integrators for Boltzmann Equation

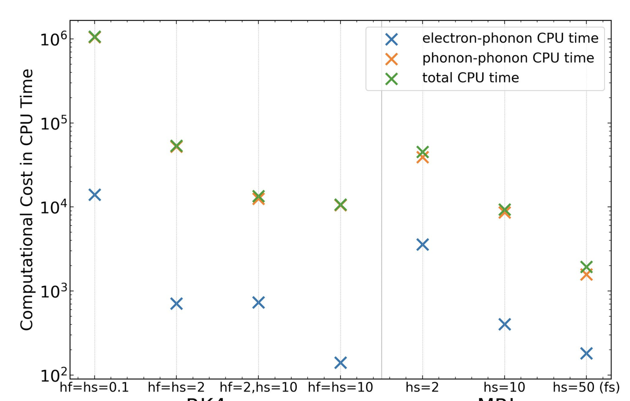
The Perturbo application in the "Death Valley" BES SciDAC simulates nonequilibrium electron dynamics with electron-phonon scattering

- Phonon-phonon interactions are VERY expensive
- Electron-phonon interactions: less expensive and on a faster time scale

We developed interfaces for Perturbo to call SUNDIALS ARKODE to enable using both adaptive single rate and multirate methods



For a given slow time step size, the multirate method gives a significant accuracy benefit over the original RK4 method for both the electron and phonon population errors, indicating that more accurate integration of the fast time scale electron-phonon interactions is critical to accuracy of the overall solution.



Computational costs for the original RK4 method and the multirate method from ARKODE show that for the same accuracy, the multirate method is much faster than the original fixed step RK4 method, e.g., compare the RK4 $h_f = h_s = 2$ fs with the MRI $h_s = 50$ fs.

In collaboration with Ivan Maliyov, Kelly Yao, and Marco Bernardi from CalTech

Adaptive Integrators for Fusion Turbulence

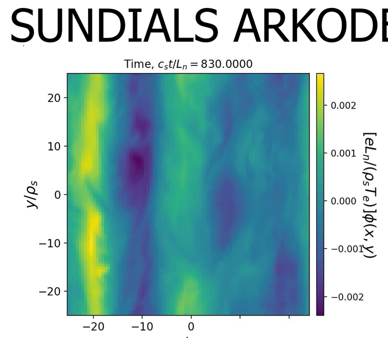
In collaboration with the MGK FES SciDAC team, we investigated time integrators for a multiscale model of ITG/ETG turbulence.

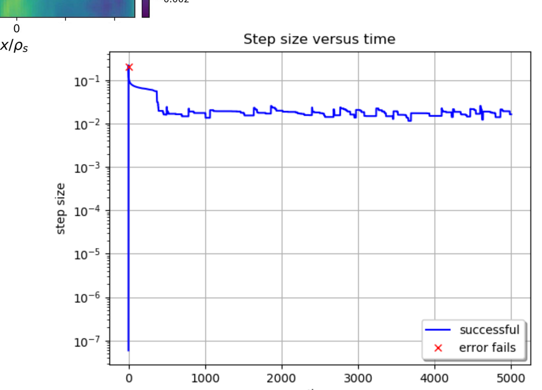
- Four 2D PDEs: ion/electron temperature and number density
- Pseudospectral discretization: evolve in the frequency domain. Differentiation and diffusion solves are "trivial," but nonlinear Poisson brackets require all-to-all communication (FFT/IFFT).
- Original: explicit RK, followed by hyperviscosity "correction"
- Explored adaptive ImEx methods from SUNDIALS ARKODE package.

Findings:

- 4th order ImEx gave best robustness and time-to-solution.
- Adaptivity selects step size to track buildup vs turbulent phases.
- Buildup phase is prone to numerical instabilities; adaptivity keeps this in check, discarding poor results

Now investigating multirate methods.





In collaboration with Darin Ernst (MIT) and Mana Francisquez (PPPL)

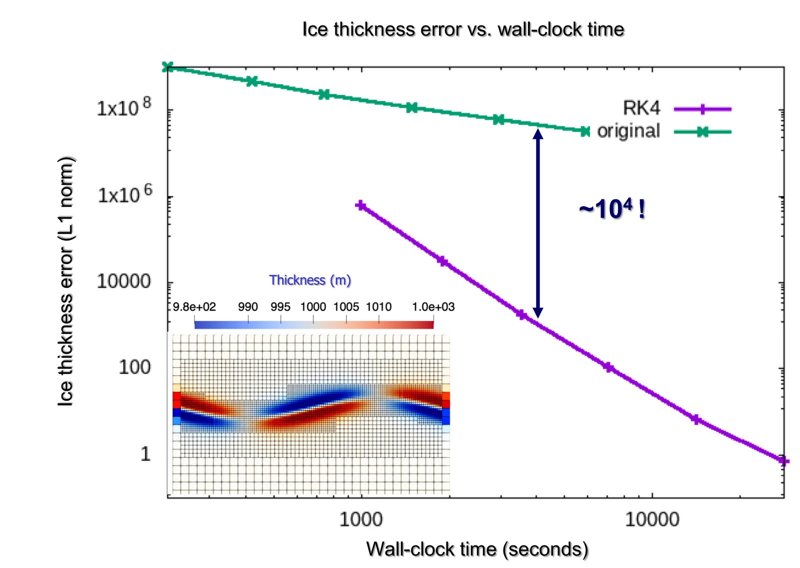
High-Order Time-Stepping for Ice Sheets

The BISICLES application simulates long-term evolution of ice sheets to predict instabilities and sea level rise

- Ice sheet modeled with an asymptotic approximation to Stokes flow
- Performance limited by poor accuracy and stability of 1st order integrator
- Linked SUNDIALS to FASTMath Chombo to enable adaptive time-stepping on AMR applications like BISICLES
- Applied high order, explicit RK from SUNDIALS ARKODE package.

Findings on "Twisty Stream" Benchmark:

- Orders of magnitude less temporal error using high order time integrators
- 35% reduction in runtime for stability-limited regimes
- Embedded error estimation simple and robust alternative to CFL-based time step selection



In collaboration with Daniel Martin and Hans Johansen of LBNL

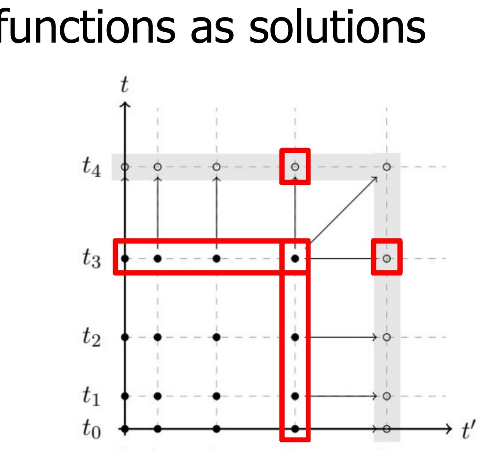
Adaptive Integrators for the Kadanoff-Baym Eqns

With the "Death Valley" BES SciDAC team, we are applying adaptive time integration methods to non-equilibrium quantum dynamical simulations

- The Kadanoff-Baym equations are a two-time system of Volterra integro-differential equations which emit a set of Green's functions as solutions

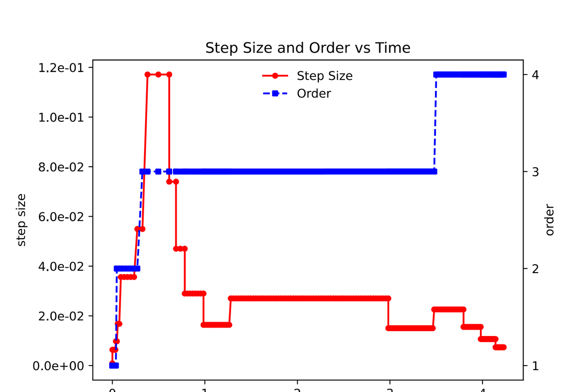
$$(\mathrm{i}\partial_t - \boldsymbol{h}_0)\,\boldsymbol{G}^<(t,t') = \int_{t_0}^{t} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^>(t,\bar{t})\boldsymbol{G}^<(\bar{t},t') + \int_{t}^{t'} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^<(t,\bar{t})\boldsymbol{G}^<(\bar{t},t') + \int_{t'}^{t_0} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^<(t,\bar{t})\boldsymbol{G}^>(\bar{t},t'),$$

$$(\mathrm{i}\partial_t - \boldsymbol{h}_0)\,\boldsymbol{G}^>(t,t') = \int_{t_0}^{t'} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^>(t,\bar{t})\boldsymbol{G}^<(\bar{t},t') + \int_{t'}^{t} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^>(t,\bar{t})\boldsymbol{G}^>(\bar{t},t') + \int_{t}^{t_0} \mathrm{d}\bar{t}\,\boldsymbol{\Sigma}^<(t,\bar{t})\boldsymbol{G}^>(\bar{t},t')$$



The system size grows with each time step

- $G^<$ and $G^>$ are Green functions, h_0 is the Hamiltonian, & Σ are nonlinear self-energies
- Interfaces the SUNDIALS CVODE integrator with the NEDyson code
- Enhanced CVODE to handle changing problem sizes and rebuilding history
- Order and step size adapt to track dynamics
- Modifications to NEDyson to advance all points on the leading edge in the (t, t') plane at once and storing values for history reconstruction



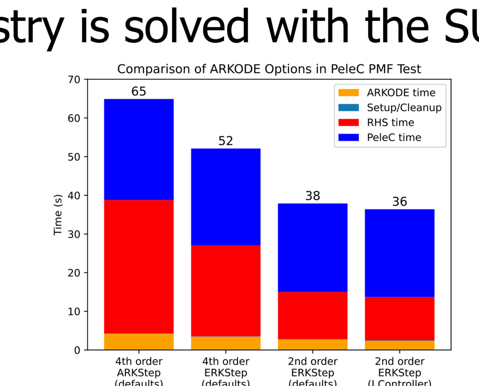
Step size and order history with CVODE BDF methods in a two-ramp KBE simulation

In collaboration with Emanuel Gull and Thomas Blommel of Univ. of MI

GPU Adaptive Integrators for Combustion

Working with the Pele reactive flow team in the Exascale Computing Project, we deployed SUNDIALS time integrators in the Pele combustion codes.

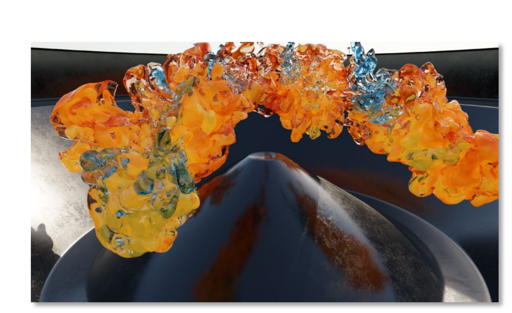
- PeleC solves the Navier-Stokes equation in the compressible regime, while PeleLM handles the low Mach number regime, both with reactive chemistry
- Both codes use operator splitting to allow for separate treatment of the fluid dynamics and the chemical reactions; chemistry is solved with the SUNDIALS CVODE integrator



Runtimes for PeleC using different ARKODE options. Saw 44% reduction in runtime w/ algorithm choices.

Results:

- Flexibility of SUNDIALS allows comparison of methods and options with relative ease
- SUNDIALS interfaces to GPU-enabled direct linear solver packages, like MAGMA, provided significant performance improvement over GMRES
- Relative time spent doing chemistry integration greatly reduced
- Scaled up to 7000 nodes of Frontier and 1B degrees of freedom



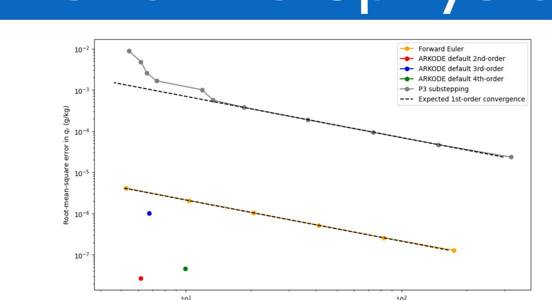
Isosurfaces of diesel fuel entering a turbulent methane-air premixture at 60 atm. High temperature pockets (seen in red and yellow) form when local kernels of diesel fuel ignite. The simulation size increases over time, growing up to 1B degrees of freedom.

In collaboration with Marc Day, Jon Rood, and Lucas Esclapez of NREL

High Order Methods in Atmospheric Microphysics

PAESCAL BER SciDAC project is improving numerics for coupled processes in microphysics

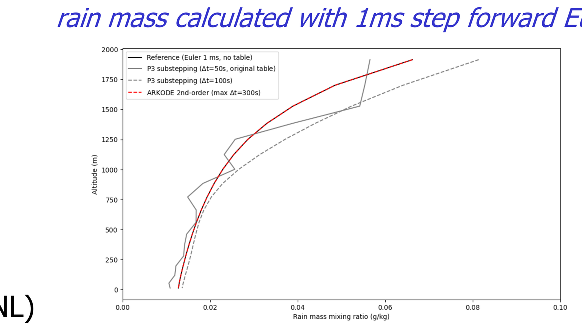
- First test code is a rainshaft model processes involving only rain and the bulk atmosphere
- Interfaced this code with SUNDIALS ARKODE to test higher order explicit integrators



Error vs time for rainshaft model. RMS error in rain mass calculated with 1ms step forward Euler.

Findings:

- For same amount of work, 2nd and 3rd order methods give more accuracy than 1st order
- *See PAESCAL microphysics poster*



In collaboration with Sean Santos & Hui Wan (PNNL) and Chris Vogl (LLNL)

Adaptive Integrators for Nuclear Physics

In collaboration with the NUCLEI NP SciDAC, deployed SUNDIALS CVODE time integrators in coupled-cluster theory (NUCCOR) and In-medium similarity renormalization group codes (IMSRG).

- CVODE enables NUCCOR with variable step *and* order methods as well as GPU capabilities for modern HPC platforms
- Exploring automatic selection of nonlinear solver (fixed-point or Newton) method to improve efficiency of IMSRG code

In collaboration with Heiko Hergert (MI State) and Zhonghao Sun (UTK)

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More Information: http://scidac5-fastmath.lbl.gov or contact Carol Woodward, LLNL, woodward6@llnl.gov, 925-424-6013

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