Time Integration for Atmospheric Physics

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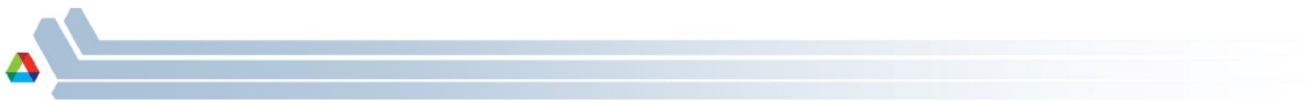
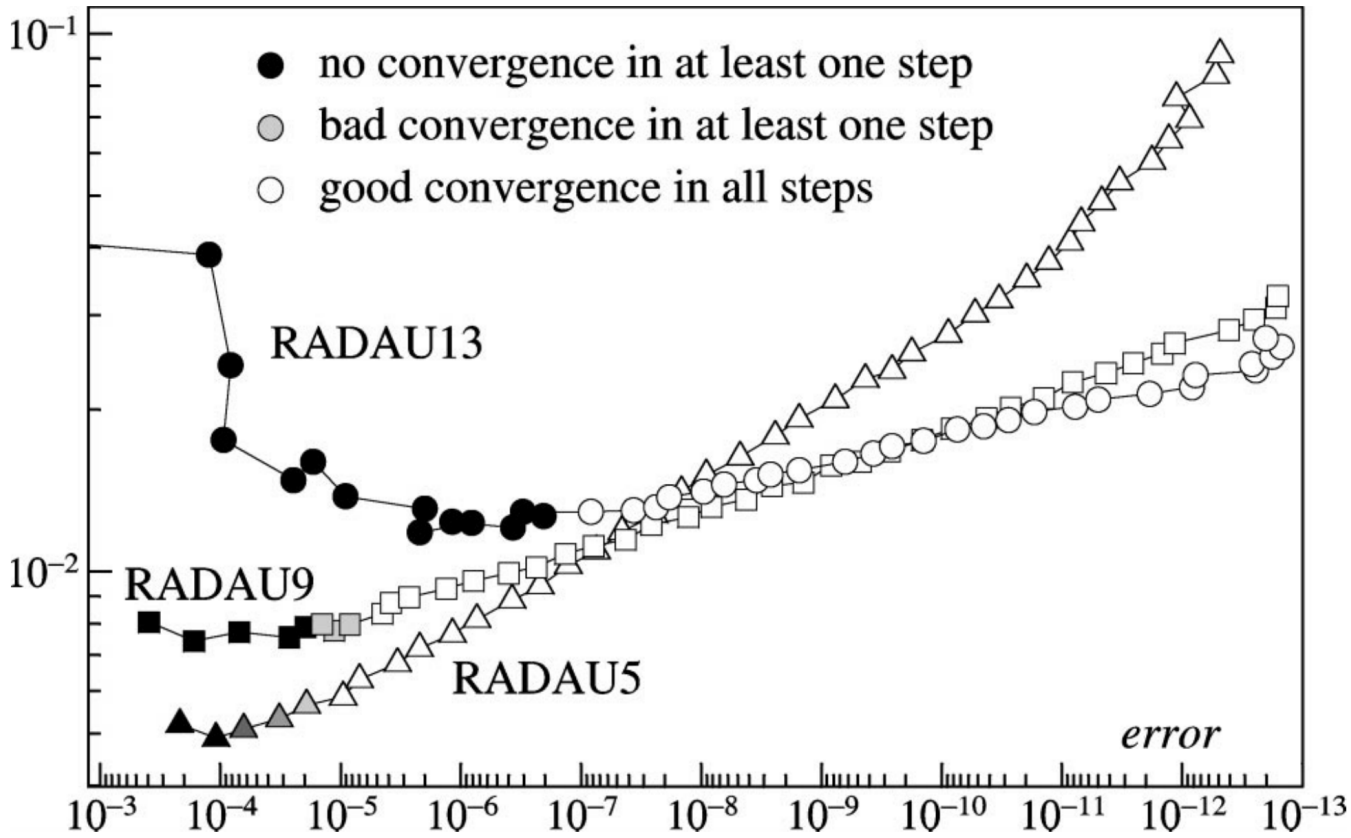
What is performance?

- Accuracy
- Model complexity
- Compute Time
- Human Time
- Cost

- Terms relevant to scientist/engineer
- No flop/s, number of elements/time steps



Work-precision diagram: *de rigueur* in ODE community



[Hairer and Wanner (1999)]

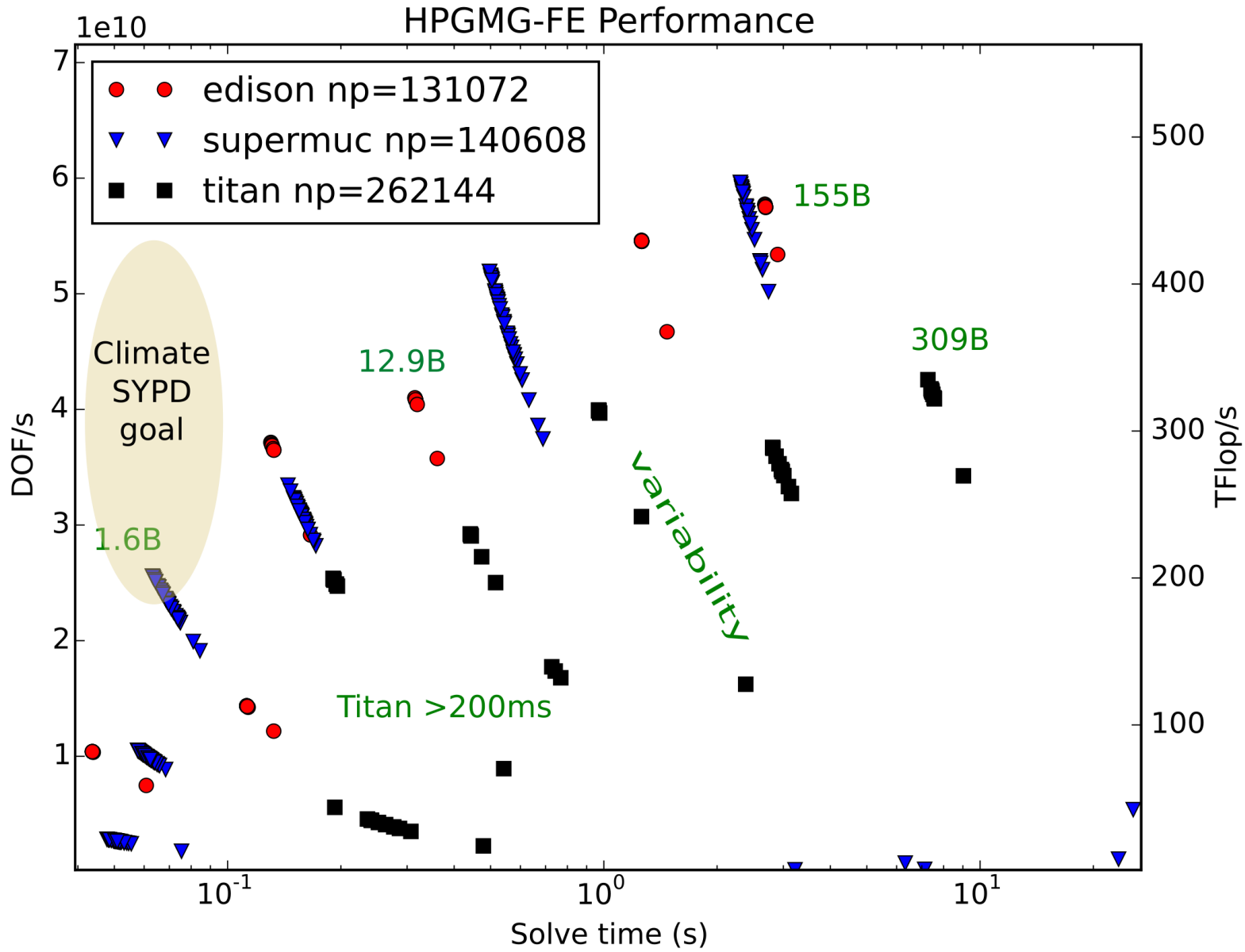
- Tests discretization, adaptivity, algebraic solvers, implementation
- No reference to number of time steps, number of grid points, etc.

Exascale Science & Engineering Demands

- Model fidelity: resolution, multi-scale, coupling
  - Transient simulation is not weak scaling: $\Delta t \sim \Delta x$
- Analysis using a sequence of forward simulations
  - Inversion, data assimilation, optimization
  - Quantify uncertainty, risk-aware decisions
- Increasing relevance $\Longrightarrow$ external requirements on time
  - Policy: 5 SYPD to inform IPCC
  - Weather, manufacturing, field studies, disaster response
- "weak scaling" [. . .] will increasingly give way to "strong scaling"

  [The International Exascale Software Project Roadmap, 2011]
- ACME @ 15 km scaling saturates at $< 10\%$ of Titan (CPU) or Mira
  - Cannot decrease Δx: SYPD would be too slow to calibrate
  - "results" would be meaningless for 50-100y predictions, a "stunt run"
- **ACME v1 goal of 5 SYPD is pure strong scaling.**
  - Many non-climate applications in same position.

HPGMG-FE on Edison, SuperMUC, Titan



What is Stiffness?

Definition (Stiffness)

A dynamical system is *stiff* if time integration efficiency is limited by stability rather than accuracy.

- Is air flow in this room stiff?
- A property of the physical system *and* quantities of interest

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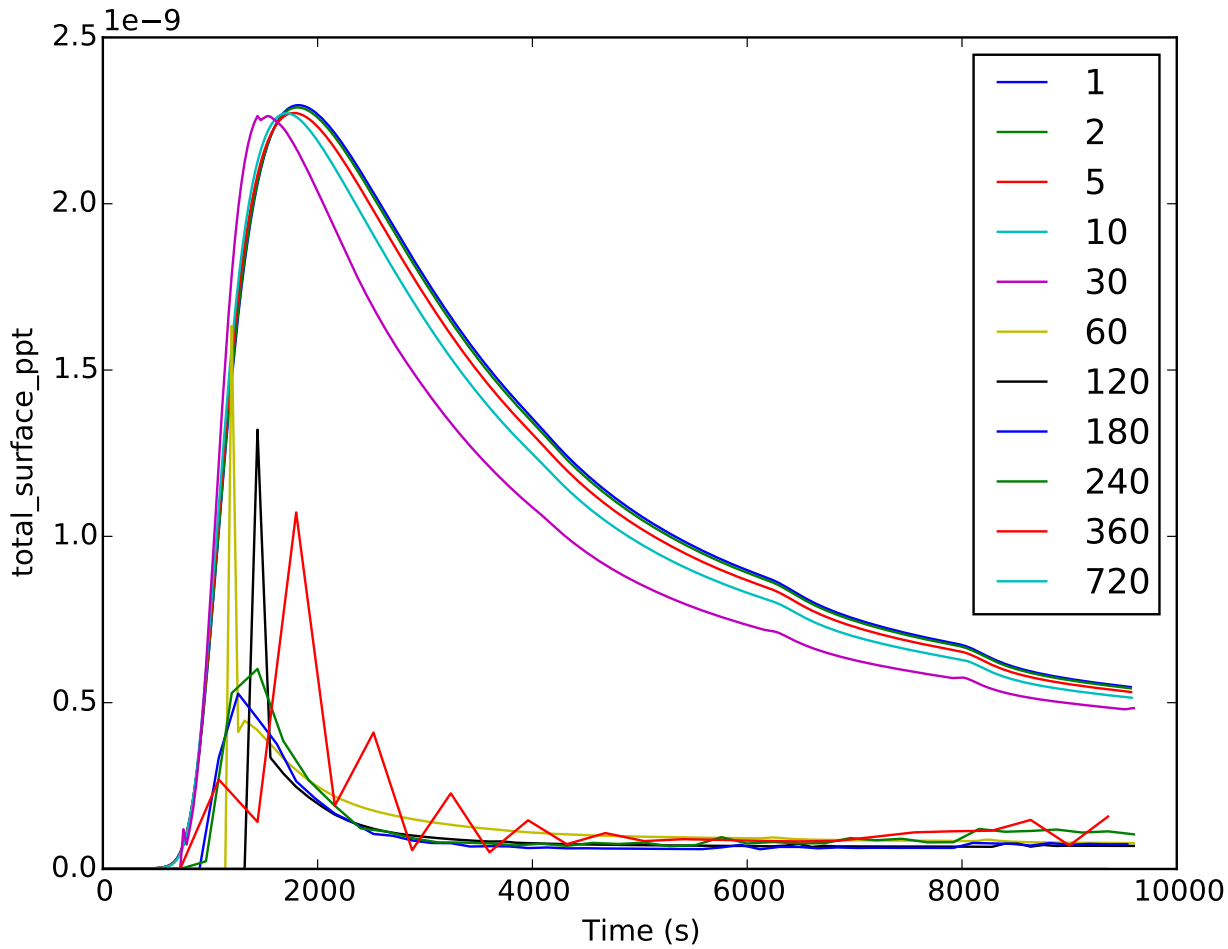
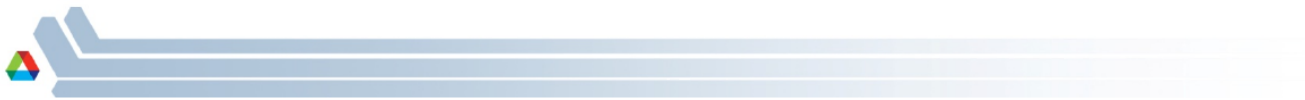
KiD: Kinematic Driver

- Shipway and Hill (UK Met Office)
- Morrison and Gettelman (NCAR) - CAM5 microphysics
- Peter Caldwell (LLNL)
- 1D and 2D mode, diagnostic velocity
- Time integration methods
  - Heavy use of splitting
  - Some implicit substeps
- State scattered among global variables
- Functions take time steps with side-effects

Accuracy of reference integrator

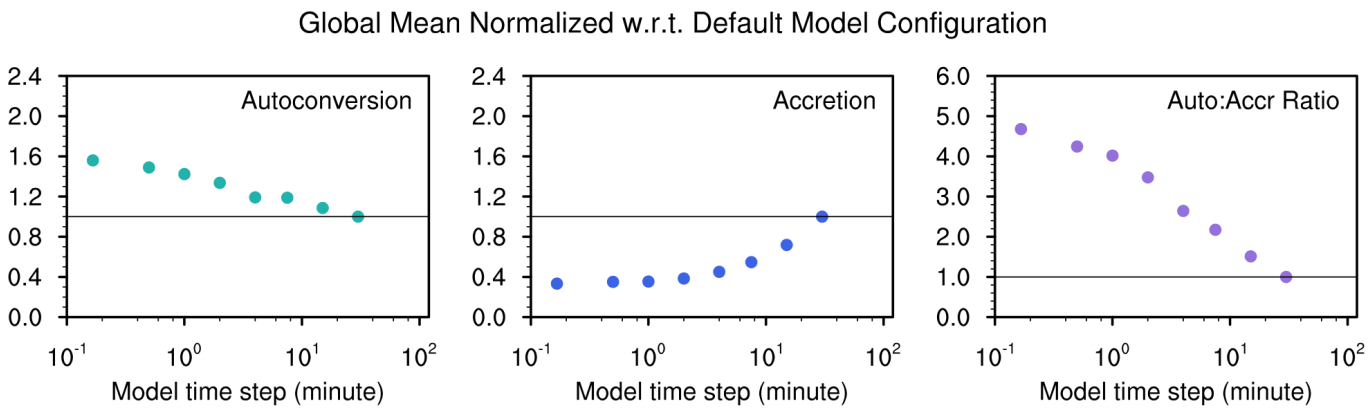


- Solution completely wrong for $\Delta t > 30s$
- Production time steps are several minutes



Calibration (c/o Caldwell)

Impact of time step on autoconversion vs accretion partitioning (from Hui)



- Parameters calibrated for systematic discretization error

IMEX time integration in PETSc

- Additive Runge-Kutta IMEX methods

$$G(t, x, \dot{x}) = F(t, x)$$

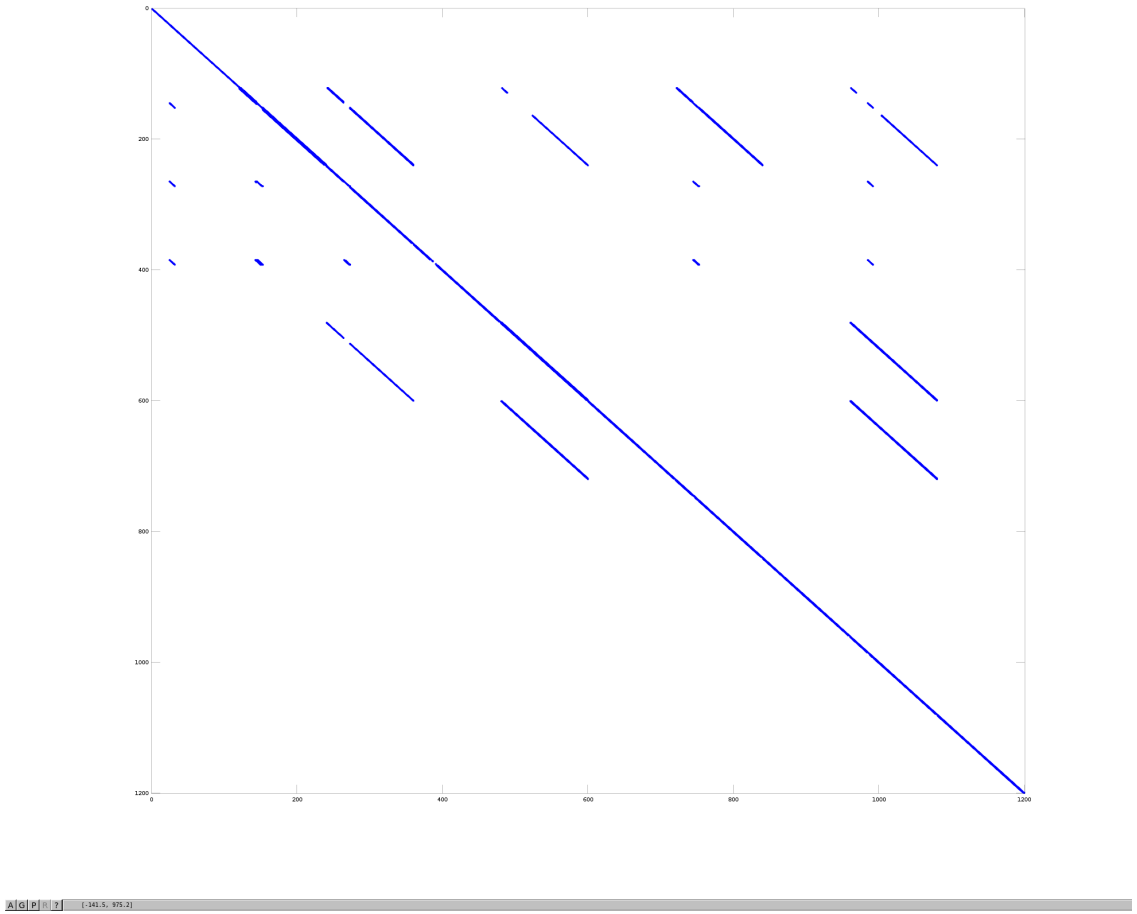
$$J_\alpha = \alpha G_{\dot{x}} + G_x$$

  - User provides:
    - `FormRHSFunction(ts,`t`,`x`,`F`,void *ctx);`
    - `FormIFunction(ts,`t`,`x`,`$\dot{x}$`,`G`,void *ctx);`
    - `FormIJacobian(ts,`t`,`x`,`$\dot{x}$`,`α`,`J`,`J_p`,mstr,void *ctx);`
  - Can have L-stable DIRK for stiff part G, SSP explicit part, etc.
  - Orders 2 through 5, embedded error estimates
  - Dense output, hot starts for Newton
  - More accurate methods if G is linear, also Rosenbrock-W
  - Can use preconditioner from classical “semi-implicit” methods
  - FAS nonlinear solves supported
  - Extensible adaptive controllers, can change order within a family
  - Easy to register new methods: `TSARKIMEXRegister()`
- Single step interface so user can have own time loop
- Same interface for Extrapolation IMEX

How to use KiD with PETSc

- Estimate $f(u)$
  1. Unpack $u(t)$ into legacy global state variables
  2. Step from t to $t+\delta t$
  3. Pack $u(t+\delta t)$ into Vec
  4. $f(u) = \left[u(t+\delta t) - u(t)\right]/\delta t$
- Side effects
- Numerical stability
  - Finite difference Jacobian
- Ill conditioning
  - Jacobian has condition number 10^{38}
  - Is 10^{-10} small or large?
  - How much is essential ill-conditioning

Sparsity



- One column: temperature, water vapor, cloud, rain, ice, snow, graupel
- Looks easy for direct solvers

Outlook

- Finite differencing twice is bad for ill-condition problems
- Quad precision would be useful (available in PETSc)
- Thou shalt non-dimensionalize
- Global state is bad
- Side-effects in residual evaluation is bad
- We can compensate for a lot on the outside
- What is essential ill-conditioning?
- Can coupled implicit/IMEX be more efficient?
- How incipient are positivity issues?
- Does the community care about accuracy?
  - Parameters calibrated to compensate for systematic bias
  - Validation expensive even if method is better