Higher Standards on the Control of Numerical Accuracy

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Editorial Policy Statement on the Control of Numerical Accuracy

A professional problem exists in the computational fluid dynamics community and also in the broader area of computational physics. Namely, there is a need for higher standards on the control of numerical accuracy.

The numerical fluid dynamics community is aware of this problem but, although individual researchers strive to control accuracy, the issue has not to our knowledge been addressed collectively and formally by any professional society of journal editorial board. The problem is certainly not unique to the JFE and came into even sharper focus at the 1980-81 AFOSRHTTM-Stanford Conference on Complex Turbulent Flows. It was a conclusion of that conference's Evaluation standards should be raised. Consequently, this journal hereby announces the following policy:

> *The Journal of Fluids Engineering will not accept for publication any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation.*

Although the formal announcement of this journal policy is new, it has been the practice of many of our conscientious reviewers. Thus the present announcement is not a change in policy so much as a clarification and standardization.

Methods are available to accomplish this task, such as

[Roache, Ghia, White (1986)]

- "it was impossible to compare the accuracy of different turbulence models, since one could not distinguish physical modeling errors from numerical errors related to the algorithm and grid."

cedure is explained."[2] Whatever the authors use will be considered in the review process, but we must make it clear that *a single calculation in a fixed grid will not be acceptable*, since it is impossible to infer an accuracy estimate from such a calculation. Also, the editors will not consider a reasonable agreement with experimental data to be sufficient proof of accuracy, especially if any adjustable parameters are involved, as in turbulence modeling.

We recognize that it can be costly to do a thorough study, and that many practical engineering calculations will continue to be performed on a single fixed grid. However, this practice is insufficient for publication in an archival journal.

Climate: science or engineering?

- Inform international policy decisions
- Water resource management
- Financial investments (e.g., reinsurance)
- Risk assessment depends on higher order statistics
- Engineering validation experience consistently finds that verification is necessary for reliability
- Rigorous validation is not feasible
  - Calibration is ad-hoc: cannot tell scientists to “forget” the last few decades to avoid over-fitting
  - Statistical variation is large, but only one observed realization

MPAS: Inconsistent discretization of Coriolis

	Rotational flow		Divergent flow	
Grid & Cells	L_∞ err	L_2 err	L_∞ err	L_2 err
Hex				
42	0.59×10^{-1}	0.34×10^{-1}	0.78×10^{-1}	0.45×10^{-1}
162	0.49×10^{-1}	0.16×10^{-1}	0.52×10^{-1}	0.18×10^{-1}
642	0.35×10^{-1}	0.69×10^{-2}	0.35×10^{-1}	0.71×10^{-2}
2562	0.29×10^{-1}	0.37×10^{-2}	0.28×10^{-1}	0.38×10^{-2}
10 242	0.23×10^{-1}	0.25×10^{-2}	0.23×10^{-1}	0.26×10^{-2}
40 962	0.23×10^{-1}	0.20×10^{-2}	0.23×10^{-1}	0.20×10^{-2}
163 842	0.23×10^{-1}	0.14×10^{-2}	0.23×10^{-1}	0.14×10^{-2}
Cube				
54	0.68×10^{-1}	0.38×10^{-1}	0.65×10^{-1}	0.23×10^{-1}
216	0.12	0.41×10^{-1}	0.85×10^{-1}	0.41×10^{-1}
864	0.14	0.29×10^{-1}	0.11	0.29×10^{-1}
3456	0.15	0.19×10^{-1}	0.13	0.20×10^{-1}
13 824	0.15	0.13×10^{-1}	0.14	0.15×10^{-1}
55 296	0.15	0.95×10^{-2}	0.15	0.11×10^{-1}
221 184	0.15	0.67×10^{-2}	0.15	0.75×10^{-2}

[Thuburn, Cotter, Dubos (2014)]

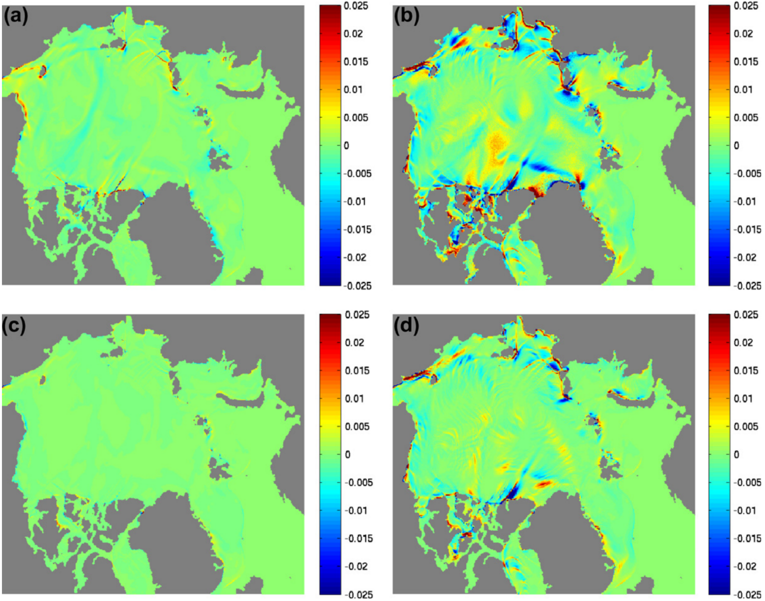
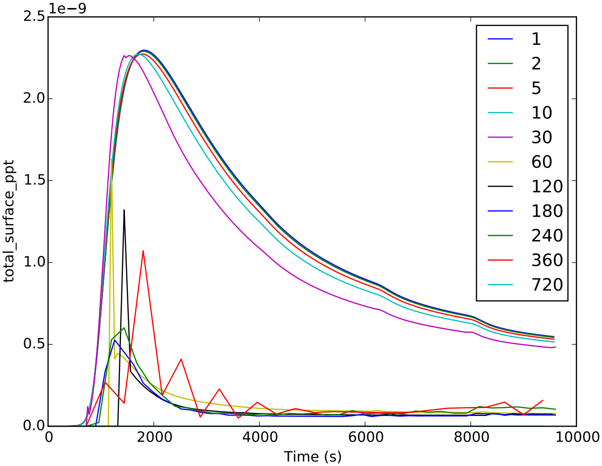


Fig. 5. Difference between the thickness field obtained with JFNK with $\gamma_{nl} = 0.5$ (a) or $\gamma_{nl} = 10^{-3}$ (c) and the reference solution. Difference between the thickness field obtained with the EVP with $N_{sub} = 120$ (b) or $N_{sub} = 1920$ (d) and the reference solution. The advective time step for the JFNK and EVP solvers is 20 min. To see the details, the thickness differences are capped to ± 2.5 cm.

KiD: Kinematic Driver

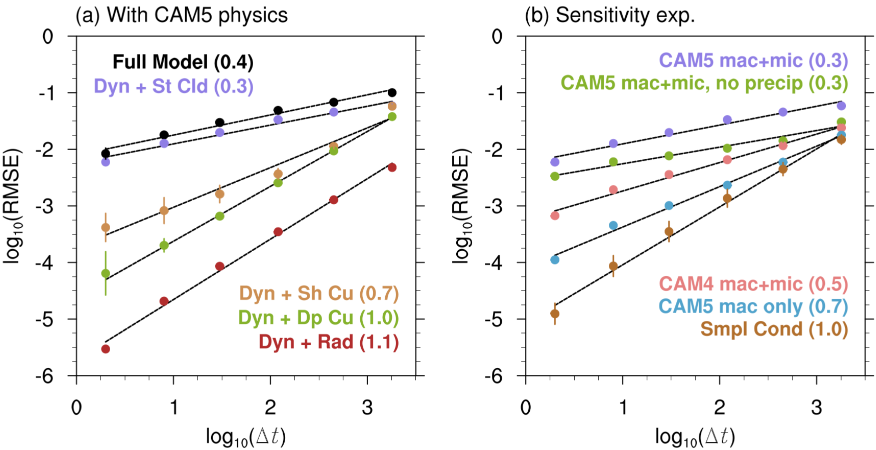
- Shipway and Hill (UK Met Office)
- Morrison and Gettelman (NCAR) - CAM5 microphysics
- Peter Caldwell (LLNL)
- 1D and 2D mode, diagnostic velocity
- Time integration methods
  - Heavy use of splitting
  - Some implicit substeps

KiD: accuracy of time integrator



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

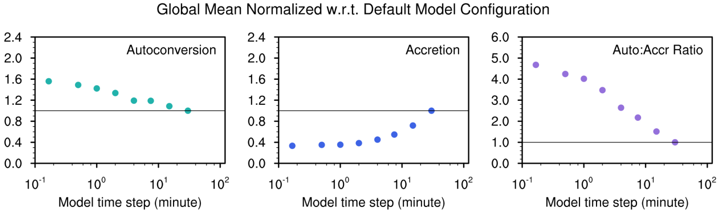
Slows convergence of global model



[Wan et al. 2015]

Calibration (c/o Caldwell)

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



- Parameters calibrated for systematic discretization error

Parameter tuning

With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.
— John von Neumann

- Over-fitting is a pathology
- *Good* subgrid models do not require (much) re-tuning parameters when Δt or Δx change
- Experimenting with new discretizations requires expensive, ad-hoc parameter re-calibration.

What to do about numerical accuracy?

- Evaluate new and existing models to distinguish modeling and numerical errors
- Improve discretizations to address deficiencies
- Formalize parameter calibration
  - especially when discretization error cannot be made small compared to modeling error
- Cannot evaluate errors in idealized scenarios (e.g., artificial viscosity turned off), then use with such terms
- Likely shift from naive splitting towards more implicit methods
  - potential improvement to algorithmic scalability and fine-grained parallelism
- May require coupler redesign (after addressing errors within each component)

Outlook: Systematic approach to numerical accuracy

- Better understanding of the underlying multiscale physics
- Convergent numerical methods
- Higher quality predictions
- Calibration more robust, reduces recalibration effort
- Improve understanding of model uncertainties