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Optimization-based property-preserving methods

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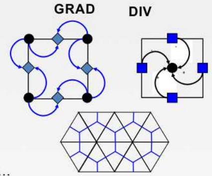
Abstract

This project has pioneered the use of optimization and control ideas for the formulation of new classes of heterogeneous and property-preserving numerical methods. Examples include optimization-based formulations for local-to-non-local and atomistic-to-continuum couplings and transmission problems. This poster focusses on application of the approach to obtain new property-preserving numerical methods.

Motivation: What do we want in a numerical method?

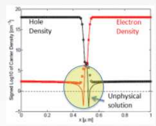
1. Stable & Accurate (Structural aspects)



- **Game changer**: **Homological techniques**:
  - FE exterior calculus (DEC), mimetic FD,…
- Typically achieved by *topological means:*
  - Careful placement of the variables on the mesh.
  - Special grid structure, e.g., topologically dual grids.
- **Challenges**:
  1. **Models that don't fit EC structure**
  2. **Stable and accurate does not imply property preserving**…

2. Preserves Physical Properties (Qualitative aspects)

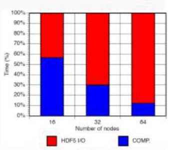
- Maximum principles, local bounds, symmetries, GCL,…
- Correlations between variables, e.g., between two passive tracers.
- **Challenges**: conventional ways to preserve these properties are either
  - **Restrictive**: Cartesian mesh, angle conditions, etc, and/or,
  - **Entangle accuracy** with the property preservation, e.g., limiters.
- **Game changer?**



Violation of physical bounds in a PN diode simulation

3. Fault-tolerant (it's a brave new world of hardware)

- Mean time between failures on the future HPC platforms is expected to decrease to just a few minutes
- Taking faster checkpoints: the most effective and possibly the only viable strategy for sustained application utilization at extreme scales(1)
- Development of "smart", property-preserving checkpointing schemes becomes imperative to avoid dramatic decreases in application utilization.



Time distribution(2) in terms of useful computation (COMP) and I/O (HDF5) for a water simulation with QMCPack.

(1) B. Schroeder and G.A. Gibson. Understanding failures in petascale computers. Journal of Physics: Conference Series, 78, 2007.

Approach

Optimization-based property-preserving methods (OBPP)

- A property-preserving OB formulation for $L(u)=f$ has 3 key building blocks

$L_h(u_h)=f_h$ — a numerical scheme to generate an optimally accurate target

$P:\mathbf{R}^n \to \mathbf{R}^m$ — a nonlinear operator describing the desired physical properties

$J:\mathbf{R}^n \to \mathbf{R}$ — a measure of target-to-state misfit

$$\underset{u_h \in \mathbf{R}^n}{\text{minimize}}\, J(u_h^T - u_h) \ \text{ subject to } \ P(u_h) \geq 0$$

OBPP separates property preservation from accuracy considerations

Mathematical and computational requirements for OBPP:

- Identify misfit measures appropriate for the problem configuration
- Translate properties into suitable constraint operators
- Ensure well-posedness of the resulting constrained optimization problem
- Develop scalable and efficient optimization algorithms which exploit the structure

Results

OBPP for scalar transport equations

$\partial_t \rho + \nabla \cdot F(\rho) = f$ — Key building block for many DOE applications: climate, shock hydro

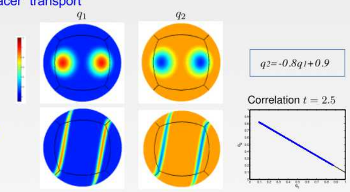
$\partial_t \rho + \nabla \cdot \rho \mathbf{v} = 0$ — conservation of "mass"

$\partial_t \rho T + \nabla \cdot \rho \mathbf{v} T = 0$ — passive "tracer" transport

⟵ sea-ice and atmosphere example

Initial tracer distributions: two linearly correlated cosine bells

Optimization formulation provably preserves linear tracer correlations



OBPP recovery

Our approach allows to embed application knowledge (governing equations, discretization, physical properties, etc.) into the compression and recovery process.

Specialization of the optimization problem

$C:\mathbf{R}^n \to \mathbf{R}^d$ — a state-to-snapshot map

$P:\mathbf{R}^n \to \mathbf{R}^m$ — a nonlinear operator describing the desired physical properties

$J:\mathbf{R}^n \to \mathbf{R}$ — a measure of target-to-state misfit

$$\underset{u \in \mathbf{R}^n}{\text{minimize}}\, J(C(u) - u_D) \ \text{ subject to } \ P(u) \geq 0$$

recovers application state u from a corrupted state u_D

Proof of principle for advection-diffusion

$M\rho^k = (\Delta t K + M)\rho^{k-1}$ — SUPG discretization

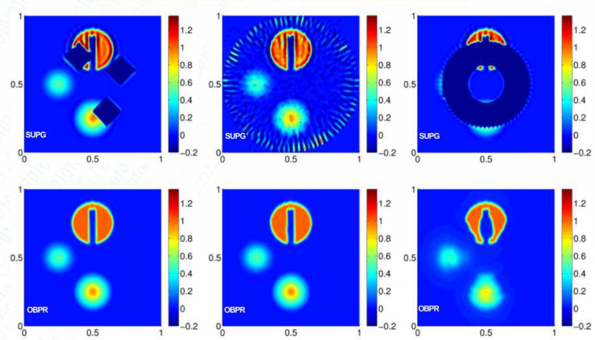
$\rho_D^k \in R^n$ — corrupted state

Q — mass matrix

$$P(\rho^k) = \begin{cases} \rho_{\min}^k \leq \rho^k \leq \rho_{\max}^k & \text{local bounds} \\ 1^T(Q\rho^k) = m & \text{mass cons.} \end{cases}$$

$C = I$ and $J(\cdot) = \|\cdot\|_{\ell_2}^2$

- Compression simulated by down sampling local bounds on coarse (1/16th) mesh and storing only total mass.
- Linear interpolation provides bounds for the recovery process
- Yields effective checkpoint compression of 87.5% (0% = no compression)
- Maintains optimal convergence rate for #1,#2, preserves mass and bounds in all cases



Failure mode ⟶

Large-yet-infrequent Entire group of spatially linked nodes fails at N/4, N/2, 3N/4.

Small-yet-frequent Random node failure at every 10th forward Euler step.

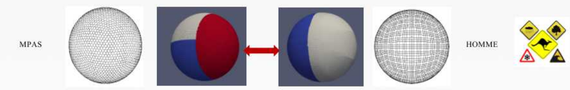
Large-and-frequent Same as case #1 but with an increased frequency of failure.

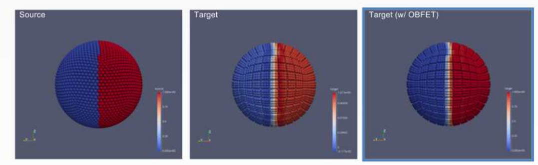
Potential Impact

- Optimization-based property-preserving recovery and compression can provide important new technologies for fault-tolerant algorithms on the next generation platforms.
- Optimization-based spectral semi-Lagrangian schemes for passive tracer transport of interest to HOMME.
- Optimization-based property-preserving remap shows significant promise for applications ranging from ALE to data transfers between separate simulation codes
- Optimization-based and heterogeneous domain decomposition coupling formulations evaluated for DOE's next generation earth system models as part of the CANGA project
- Optimization-based approach demonstrated as an effective way to couple separate simulation codes (Albany + Peridigm) to implement a local-to-nonlocal simulation capability.

Synergy

- **OBPP remap adopted in CANGA for data transfers between codes**





- **OBPP can drive research in new structure-exploiting optimization algorithms.**
- **Translation of properties into constraint operators for more complex sets of governing equations can provide additional research drivers for recent work on invariant domains for PDEs.**

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