Title: Discontinuous collocation methods and self-force applications

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Abstract: Numerical simulations of extereme mass ratio inspirals face several computational challenges. We present a new approach to evolving partial differential equations occurring in black hole perturbation theory and calculations of the self-force acting on point particles orbiting supermassive black holes. Such equations are distributionally sourced, and standard numerical methods, such as finite-difference or spectral methods, face difficulties associated with approximating discontinuous functions. However, in the self-force problem we typically have access to full a-priori information about the local structure of the discontinuity at the particle. Using this information, we show that high-order accuracy can be recovered by adding to the Lagrange interpolation formula a linear combination of certain jump amplitudes. We construct discontinuous spatial and temporal discretizations by operating on the corrected Lagrange formula. In a method-of-lines framework, this provides a simple and efficient method of solving time-dependent partial differential equations, without loss of accuracy near moving singularities or discontinuities. This method is well-suited for the problem of time-domain reconstruction of the metric perturbation via the Teukolsky or Regge-Wheeler-Zerilli formalisms. Parallel implementations on modern CPU and GPU architectures are discussed.

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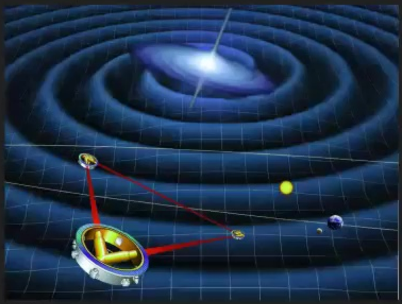
DISCONTINUOUS TIME-SYMMETRIC METHODS AND SELF-FORCE APPLICATIONS

Capra 24, Perimeter Institute, June 7-11, 2021

EMRIs – COMPUTATIONAL CHALLENGES



- EMRIs will spend months/years in LISA band, instead of the few seconds/milliseconds inspirals spend in LIGO band.
- Disparate mass/length scales. CFL condition restricts time-step.
- EMRIs computationally intractable for traditional numerical relativity.
- For perturbations in Schwarzschild spacetime, linearized Einstein equations reduce to the Bardeen-Press (or Regge-Wheeler-Zerilli) equations.
- Computing GSF in the time domain requires solving PDEs with with distributional sources. Discontinuous discretization (in space+time), and methods for long-time evolution.

1+1 BARDEEN-PRESS EQUATION

- Bardeen-Press equation

$$[(\nabla_a + s\Gamma_a)(\nabla^a + s\Gamma_a) + V_l^s(x)]\psi_{lm}^s(t,x) = 0$$

- Modal (spin-weighted spherical harmonic) expansion in θ, ϕ
- Nodal (discontinuous collocation) method in $x = r^\star$
- Symmetric (2-point Taylor or Hermite) method in t

1+1 BARDEEN-PRESS EQUATION

- Bardeen-Press equation

$$[(\nabla_a + s\Gamma_a)(\nabla^a + s\Gamma_a) + V_l^s(x)]\psi_{lm}^s(t,x) = 0$$

$$S = \int \sqrt{-\eta}\, dtdx\, [(\partial_a + s\Gamma_a)\,\psi^{(-s)}\,\eta^{ab}\,(\partial_b + s\Gamma_b)\,\psi^{(s)} + V_l^s\,\psi^{(-s)}\psi^{(s)}]$$

$$T_{ab} = (\partial_a - s\Gamma_a)\psi^{(-s)}\partial_b\psi^{(s)} + (\partial_a + s\Gamma_a)\psi^{(s)}\partial_b\psi^{(-s)} + \eta_{ab}\mathscr{L}$$

1+1 REGGE-WHEELER-ZERILLI EQUATION

- Regge-Wheeler-Zerilli equation

$$[\nabla_a \nabla^a + V_l^s(x)]\psi_{lm}^s(t,x) = 0$$

$$S = \int \sqrt{-\eta}\, dtdx\, (\partial_a \psi^\star \eta^{ab} \partial_b \psi + V_l^s \psi^\star \psi)$$

$$T_{ab} = \partial_a \psi^\star \partial_b \psi + \partial_a \psi \partial_b \psi^\star + \eta_{ab} \mathscr{L}$$

1+1 REGGE-WHEELER-ZERILLI EQUATION

- U(1) gauge symmetry $(\psi \to e^{i\alpha}\psi)$ is Noether-related to conserved current:

$$J^a = i\sqrt{-\eta}(\psi^\star \partial^a \psi - \psi \partial^a \psi^\star)$$

- Poincaré transformations give rise to "Ehrenfest theorem":

$$\frac{d}{dt}\int_\Sigma \sqrt{-\eta}\, dx\, k^a T^t_a = -\int_\Sigma \sqrt{-\eta}\, dx\, \psi^\star\, £_k V\, \psi$$

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$$\frac{d}{dt}\langle p \rangle = -\langle \partial_x V \rangle \qquad \frac{d}{dt}\langle E \rangle = \langle \partial_t V \rangle \qquad \frac{d}{dt}\langle t\, p - x\, E \rangle = -\langle (t\partial_x + x\partial_t) V \rangle$$

1+1 CANONICAL EQUATIONS

- RWZ action

$$S = \int \sqrt{-\eta}\, dtdx\, (\eta^{ab}\, \partial_a \psi^\star\, \partial_b \psi + V_l^s\, \psi^\star \psi)$$

- Hamiltonian

$$\mathscr{H} = \frac{\pi^\star \pi}{\sqrt{-\eta}\,\eta^{tt}} + \sqrt{-\eta}\,(\eta^{xx}\,\partial_x \psi^\star\, \partial_x \psi - V_l^s\, \psi^\star \psi)$$

- Canonical RWZ equation

$$\partial_t \psi = -\frac{\pi}{\sqrt{-\eta}\eta^{tt}}, \quad \partial_t \pi = \partial_x(\sqrt{-\eta}\,\eta^{xx}\,\partial_x \psi) - \sqrt{-\eta} V_l^s\, \psi$$

SYMPLECTIC STRUCTURE

- The RWZ Hamiltonian gives rise to a conserved symplectic structure

$$\Omega[(\psi_1, \pi_1), (\psi_2, \pi_2)] = \int_\Sigma (\pi_1 \psi_2 - \pi_2 \psi_1)$$

- Analogous expressions hold for GR and the Teukolsky equation
  Crnkovic & Witten, 1986
  Prabhu & Wald, CQG 35, 235004, 2018
  Green, Hollands & Zimmerman, CQG 37, 075001, 2020

- Theorem 1: Hermite integration preserves the symplectic structure for quadratic Hamiltonians
  Theorem 2: Hermite integration preserves energy & U(1) charge and for quadratic Hamiltonians

METHOD OF LINES

- Reduce to first-order in time. Discretize U, L in space. PDE evolved as coupled ODE system in time

$$\frac{d\mathbf{U}}{dt} = \mathbf{L}\mathbf{U}$$

- Apply fundamental theorem of calculus and discretize in time

$$\mathbf{U}^{n+1} - \mathbf{U}^{n} = \int_{t_n}^{t_{n+1}} dt\, \mathbf{L}\mathbf{U}(t)$$

- 1-point Taylor expansion

$$\mathbf{U}^{n+1} \simeq \left(\mathbf{I} + \Delta t\mathbf{L} + \frac{(\Delta t\mathbf{L})^2}{2!} + \frac{(\Delta t\mathbf{L})^3}{3!} + \frac{(\Delta t\mathbf{L})^4}{4!} + \dots\right)\mathbf{U}^{n}$$

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- Apply fundamental theorem of calculus and discretize in time

$$\mathbf{U}^{n+1} - \mathbf{U}^{n} = \int_{t_n}^{t_{n+1}} dt\, \mathbf{L}\mathbf{U}(t)$$

- 2-point Taylor expansion (Hermite integration)

$$\left(\mathbf{I} - \frac{\Delta t\mathbf{L}}{2} + \frac{(\Delta t\mathbf{L})^2}{12} + \ldots\right)\mathbf{U}^{n+1} \simeq \left(\mathbf{I} + \frac{\Delta t\mathbf{L}}{2} + \frac{(\Delta t\mathbf{L})^2}{12} + \ldots\right)\mathbf{U}^{n}$$

METHOD OF LINES

- Reduce to first-order in time. Discretize U, L in space. PDE evolved as coupled ODE system in time

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$$\mathbf{U}^{n+1} - \mathbf{U}^{n} = \int_{t_n}^{t_{n+1}} dt\, \mathbf{L}\mathbf{U}(t)$$

- 2-point Taylor expansion (Hermite integration)

$$\mathbf{U}^{n+1} \simeq \left(\mathbf{I} - \frac{\Delta t \mathbf{L}}{2} + \frac{(\Delta t \mathbf{L})^2}{12} + \dots\right)^{-1} \left(\mathbf{I} + \frac{\Delta t \mathbf{L}}{2} + \frac{(\Delta t \mathbf{L})^2}{12} + \dots\right) \mathbf{U}^{n}$$

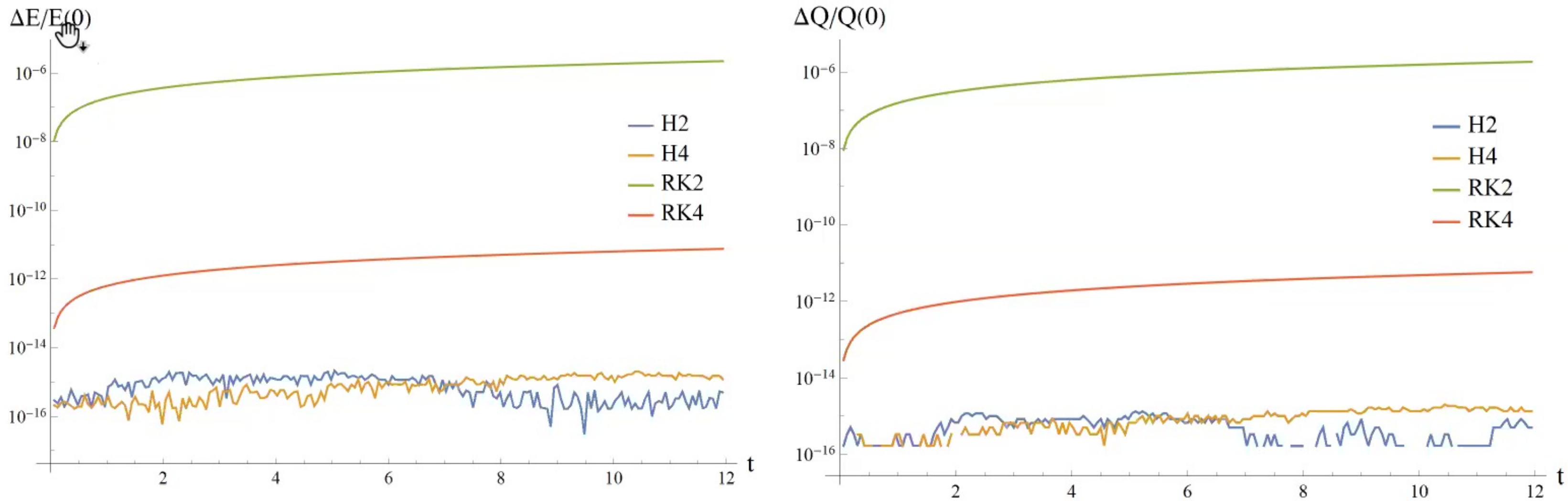
TIME-SYMMETRIC INTEGRATION IS SYMPLECTIC

- Theorem 1 proof: For quadratic Hamiltonians, a time step via Hermite integration amounts to a canonical transformation:

$$J = \frac{\partial(\psi^{n+1}, \pi^{n+1})}{\partial(\psi^{n}, \pi^{n})} = 1$$

- RK time steps fail to preserve the Jacobian and are non-canonical.

TIME-SYMMETRIC INTEGRATION PRESERVES NOETHER CHARGES



CONCLUSIONS

- Explicit methods based on 1-point Taylor expansion (e.g. Runge-Kutta) are not time-symmetric. Conditionally stable. Noether symmetries and symplectic structure violated. Simulated EMRIs lose energy to bad numerics (instead of gravitational radiation).
- Implicit methods based on 2-point Taylor expansion (Hermite integration) are time-symmetric. Unconditionally stable. Implicit methods do not incur extra cost for linear PDEs (matrix pre-inversion). Energy, U(1) charge and symplectic structure conserved. Highly desirable features for long-time numerical evolution of EMRIs.
- Can be generalized to arbitrarily high order and to discontinuous problems (method of undetermined coefficients).

C. Markakis et al. CQG 38 075031 (2021)
C. Markakis et al. [arXiv:1901.09967]

TIME-SYMMETRIC INTEGRATION PRESERVES NOETHER CHARGES