

Computational Physics

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CS 530: High Performance Computing, Spring 2024

Why do we need computers to do physics?

An Illuminating Example - 2-Body Problem

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2} \hat{r}$$

$$\sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i$$

- 2 masses
- 1 unique force
- 2 equations of motion in 3 dimensions
- 6 coupled 2nd-order ordinary differential equations

An Illuminating Example - 3-Body Problem

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2} \hat{r}$$

$$\sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i$$

- 3 masses
- 3 unique forces
- 3 equations of motion in 3 dimensions
- 9 coupled 2nd-order ordinary differential equations

An Illuminating Example - “All”-Body Problem

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2} \hat{r}$$

$$\sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i$$

- 1.24 trillion masses
- 7.688×10^{23} unique forces
- 1.24 trillion equations of motion in 3 dimensions [Cosmological N-Body Simulation\[22\]](#)
- 3.72 trillion coupled 2nd-order ordinary differential equations

Remark

Given the position and velocity of and the forces acting on an object, the motion of that object is completely determined.

- Everyday physics can be completely described by Newton's 2nd Law.

$$\underbrace{\sum_i \mathbf{F}_i = m\ddot{\mathbf{r}}}_{\text{Equation of Motion}} \quad (1)$$

- [1] G. Smith
(<https://physics.stackexchange.com/users/199630/g-smith>).
Difficulty of numerically solving Einstein equations. Physics Stack
Exchange. URL:<https://physics.stackexchange.com/q/443754>
(version: 2018-11-28). eprint:
<https://physics.stackexchange.com/q/443754>. URL:
<https://physics.stackexchange.com/q/443754>.
- [2] B. P. Abbott et al. "Observation of Gravitational Waves from a
Binary Black Hole Merger". In: *Phys. Rev. Lett.* 116 (6 Feb. 2016),
p. 061102. DOI: [10.1103/PhysRevLett.116.061102](https://doi.org/10.1103/PhysRevLett.116.061102). URL: <https://link.aps.org/doi/10.1103/PhysRevLett.116.061102>.

- [3] Tomas Andrade et al. “GRChombo: An adaptable numerical relativity code for fundamental physics”. In: *Journal of Open Source Software* 6.68 (2021), p. 3703. DOI: [10.21105/joss.03703](https://doi.org/10.21105/joss.03703). URL: <https://doi.org/10.21105/joss.03703>.
- [4] Richard Arnowitt, Stanley Deser, and Charles W. Misner. “Republication of: The dynamics of general relativity”. In: *General Relativity and Gravitation* 40.9 (Aug. 2008), pp. 1997–2027. ISSN: 1572-9532. DOI: [10.1007/s10714-008-0661-1](https://doi.org/10.1007/s10714-008-0661-1). URL: <http://dx.doi.org/10.1007/s10714-008-0661-1>.

- [5] Thomas W. Baumgarte and Stuart L. Shapiro. “Numerical integration of Einstein’s field equations”. In: *Phys. Rev. D* 59 (2 Dec. 1998), p. 024007. DOI: [10.1103/PhysRevD.59.024007](https://doi.org/10.1103/PhysRevD.59.024007). URL: <https://link.aps.org/doi/10.1103/PhysRevD.59.024007>.
- [6] Thomas W. Baumgarte and Stuart L. Shapiro. *Numerical Relativity: Starting from Scratch*. Cambridge University Press, 2021. DOI: [10.1017/9781108933445](https://doi.org/10.1017/9781108933445).
- [7] Valerie Beale and Nathan Chapman. “Distance and Plate Separation Dependence of Fringing Fields of Parallel Plate Capacitors”. In: (2019).

- [8] Abhijit Biswas and Krishnan Mani. “Relativistic perihelion precession of orbits of Venus and the Earth”. In: *Open Physics* 6.3 (2008), pp. 754–758. DOI: [doi:10.2478/s11534-008-0081-6](https://doi.org/10.2478/s11534-008-0081-6). URL: <https://doi.org/10.2478/s11534-008-0081-6>.
- [9] S. Blanes and P.C. Moan. “Practical symplectic partitioned Runge–Kutta and Runge–Kutta–Nyström methods”. In: *Journal of Computational and Applied Mathematics* 142.2 (2002), pp. 313–330. ISSN: 0377-0427. DOI: [https://doi.org/10.1016/S0377-0427\(01\)00492-7](https://doi.org/10.1016/S0377-0427(01)00492-7). URL: <https://www.sciencedirect.com/science/article/pii/S0377042701004927>.

- [10] Nathan Chapman. *A Toy Model of the Interaction between Caffeine and Stomach Acid*. 2023.
- [11] Nathan Chapman. “Effects of Eccentricity on the Precession of Orbital Periapsides due to General Relativity in the Weak Field Limit”. In: (June 2019). eprint: [\url{https://github.com/NonDairyNeutrino/ug_computation/blob/1e8f14936b1d7f5ddd2cd29961eee56ba7820a30/computational_physics/Weak_Field_GR_Eccentricity_Effects/Weak_Field_GR_Eccentricity_Effects.pdf}](https://github.com/NonDairyNeutrino/ug_computation/blob/1e8f14936b1d7f5ddd2cd29961eee56ba7820a30/computational_physics/Weak_Field_GR_Eccentricity_Effects/Weak_Field_GR_Eccentricity_Effects.pdf).
- [12] Nathan Chapman. “Effects of eccentricity on the precession of orbital periapsides due to General Relativity in the weak field limit”. In: (2019).

- [13] Nathan Chapman. “Leading Order Gravitational Wave Frequencies from Short-Term Post-Newtonian Orbits via Fourth-Order Symplectic Integration”. In: (2022).
- [14] Katy Clough et al. “GRChombo: Numerical relativity with adaptive mesh refinement”. In: *Classical and Quantum Gravity* 32.24 (Dec. 2015), p. 245011. DOI: 10.1088/0264-9381/32/24/245011. URL: <https://dx.doi.org/10.1088/0264-9381/32/24/245011>.
- [15] C.J. Cramer. *Essentials of Computational Chemistry: Theories and Models*. Wiley, 2013. ISBN: 9781118712276. URL: <https://books.google.com/books?id=k4R6cf7I7q0C>.

- [16] A. Einstein. “Die Grundlage der allgemeinen Relativitätstheorie”. In: *Annalen der Physik* 354.7 (1916), pp. 769–822. DOI: <https://doi.org/10.1002/andp.19163540702>. eprint: <https://onlinelibrary.wiley.com/doi/pdf/10.1002/andp.19163540702>. URL: <https://onlinelibrary.wiley.com/doi/abs/10.1002/andp.19163540702>.
- [17] A. Einstein, L. Infeld, and B. Hoffmann. “The Gravitational Equations and the Problem of Motion”. In: *Annals of Mathematics* 39.1 (1938), pp. 65–100. ISSN: 0003486X. URL: <http://www.jstor.org/stable/1968714> (visited on 11/29/2022).

- [18] Albert Einstein. “On the electrodynamics of moving bodies”. In: (1905).
- [19] Albert Einstein et al. “The foundation of the general theory of relativity”. In: *Annalen Phys* 49.7 (1916), pp. 769–822.
- [20] D.J. Griffiths. *Introduction to Electrodynamics*. Cambridge University Press, 2017. ISBN: 9781108357142. URL: <https://books.google.com/books?id=Kh4xDwAAQBAJ>.
- [21] David Hanson et al. “8.3: Hartree-Fock Equations are Solved by the Self-Consistent Field Method”. In: LibreTexts.org. Chap. 8: Multielectron Atoms.

- [22] Katrin Heitmann et al. “The Last Journey. I. An Extreme-scale Simulation on the Mira Supercomputer”. In: *The Astrophysical Journal Supplement Series* 252.2 (Jan. 2021), p. 19. DOI: [10.3847/1538-4365/abcc67](https://doi.org/10.3847/1538-4365/abcc67). URL: <https://dx.doi.org/10.3847/1538-4365/abcc67>.
- [23] Oliver James et al. “Gravitational lensing by spinning black holes in astrophysics, and in the movie Interstellar”. In: *Classical and Quantum Gravity* 32.6 (Feb. 2015), p. 065001. DOI: [10.1088/0264-9381/32/6/065001](https://doi.org/10.1088/0264-9381/32/6/065001). URL: <https://dx.doi.org/10.1088/0264-9381/32/6/065001>.

- [24] C Körber et al. “A primer to numerical simulations: the perihelion motion of Mercury”. In: *Physics Education* 53.5 (June 2018), p. 055007. DOI: [10.1088/1361-6552/aac487](https://doi.org/10.1088/1361-6552/aac487). URL: <https://dx.doi.org/10.1088/1361-6552/aac487>.
- [25] Christopher Körber et al. “A primer to numerical simulations: the perihelion motion of Mercury”. In: *Physics Education* 53.5 (2018), p. 055007.
- [26] MIT Game Lab. *OpenRelativity*. Online. 2012. URL: <http://gamelab.mit.edu/research/openrelativity/>.
- [27] Zhi-Han Li, Chen-Qi Li, and Long-Gang Pang. *Solving Einstein equations using deep learning*. 2023. arXiv: 2309.07397 [gr-qc].

- [28] Jacques-Louis Lions, Yvon Maday, and Gabriel Turinici. “A “parareal” in time discretization of PDEs”. In: *Comptes Rendus de l’Académie des Sciences - Series I - Mathematics* 332.7 (2001), pp. 661–668. ISSN: 0764-4442. DOI: [https://doi.org/10.1016/S0764-4442\(00\)01793-6](https://doi.org/10.1016/S0764-4442(00)01793-6). URL: <https://www.sciencedirect.com/science/article/pii/S0764444200017936>.
- [29] C.W. Misner et al. *Gravitation*. Princeton University Press, 2017. ISBN: 9781400889099. URL: <https://books.google.com/books?id=zAAuDwAAQBAJ>.
- [30] M Misner, K. Thorne, and J. Wheeler. *Gravitation*. Freeman, 1972.

- [31] Hanno Rein, Garrett Brown, and Daniel Tamayo. “On the accuracy of symplectic integrators for secularly evolving planetary systems”. In: *Monthly Notices of the Royal Astronomical Society* 490.4 (Oct. 2019), pp. 5122–5133. ISSN: 0035-8711. DOI: [10.1093/mnras/stz2942](https://doi.org/10.1093/mnras/stz2942). eprint: <https://academic.oup.com/mnras/article-pdf/490/4/5122/30725851/stz2942.pdf>. URL: <https://doi.org/10.1093/mnras/stz2942>.
- [32] Dhananjay Saikumar. *Parallel N-body simulations of planetary systems: a direct approach*. 2022. arXiv: 2208.13562 [astro-ph.EP].

- [33] Simon, J.-L. et al. “New analytical planetary theories VSOP2013 and TOP2013”. In: *A&A* 557 (2013), A49. DOI: [10.1051/0004-6361/201321843](https://doi.org/10.1051/0004-6361/201321843). URL: <https://doi.org/10.1051/0004-6361/201321843>.
- [34] Simulating eXtreme Spacetimes. *Two Black Holes Merge into One*. Youtube. 2016. URL: https://youtu.be/I_88S8DWbcU?si=fKwrNrQl8TBqaPIg.
- [35] J.R. Taylor. *Classical Mechanics*. G - Reference, Information and Interdisciplinary Subjects Series. University Science Books, 2005. ISBN: 9781891389221. URL: <https://books.google.com/books?id=P1kCtNr-pJsC>.

- [36] Jack Wisdom and Matthew Holman. “Symplectic maps for the N-body problem.”. In: *aj* 102 (Oct. 1991), pp. 1528–1538. DOI: [10.1086/115978](https://doi.org/10.1086/115978).
- [37] Haruo Yoshida. “Construction of higher order symplectic integrators”. In: *Physics Letters A* 150.5 (1990), pp. 262–268. ISSN: 0375-9601. DOI: [https://doi.org/10.1016/0375-9601\(90\)90092-3](https://doi.org/10.1016/0375-9601(90)90092-3). URL: <https://www.sciencedirect.com/science/article/pii/0375960190900923>.