Computational Physics

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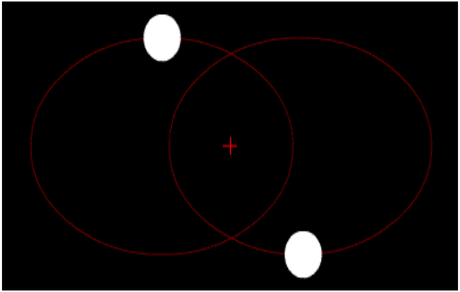
Why do we need computers to do physics?

An Illuminating Example - 2-Body Problem

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2}\hat{r} \qquad \sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i \tag{1}$$

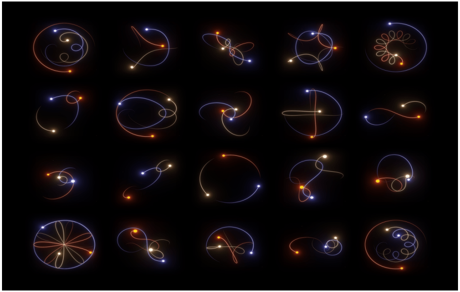
- 2 masses
- 1 unique force
- 2 equations of motion in 3 dimensions
- 6 coupled 2nd-order ordinary differential equations



An Illuminating Example - 3-Body Problem

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2}\hat{r} \qquad \sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i \tag{2}$$

- 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

$$\vec{F}_{ij} = \frac{Gm_i m_j}{r_{ij}^2}\hat{r} \qquad \sum_j \vec{F}_{ij} = m_i \ddot{\vec{r}}_i \tag{3}$$

- 1.24 trillion masses
- 7.688×10^{23} unique forces
- 1.24 trillion equations of motion in 3 dimensions
- 3.72 trillion coupled 2nd-order ordinary differential equations

Cosmological N-Body Simulation[22]

Where do we need computers to do physics?

Problems in Computational Physics

Pillars of Physics		Computational Applications
• Classical Mechanics	$\longrightarrow$	N-Body Simulations & Fluid Dynamics

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Relativity	$\longrightarrow$	Mercury's Perihelion & Black Hole Ray Tracing

Classical Mechanics

Classical Mechanics - Mathematical Model

Remark

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

- The *equation of motion*: $\sum_i \mathbf{F}_i = m\ddot{\mathbf{r}}$
- 2nd-order
- Ordinary
- 3 dimensions

Classical Mechanics - 3-Body Equations of Motion

$$\frac{Gm_2}{((x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2)^{3/2}}\begin{bmatrix}x_2-x_1\\y_2-y_1\\z_2-z_1\end{bmatrix}+\frac{Gm_3}{((x_1-x_3)^2+(y_1-y_3)^2+(z_1-z_3)^2)^{3/2}}\begin{bmatrix}x_3-x_1\\y_3-y_1\\z_3-z_1\end{bmatrix}=\begin{bmatrix}\ddot{x_1}\\\ddot{y_1}\\\ddot{z_1}\end{bmatrix} \tag{4}$$

$$\frac{Gm_1}{((x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2)^{3/2}}\begin{bmatrix}x_1-x_2\\y_1-y_2\\z_1-z_2\end{bmatrix}+\frac{Gm_3}{((x_2-x_3)^2+(y_2-y_3)^2+(z_2-z_3)^2)^{3/2}}\begin{bmatrix}x_3-x_2\\y_3-y_2\\z_3-z_2\end{bmatrix}=\begin{bmatrix}\ddot{x_2}\\\ddot{y_2}\\\ddot{z_2}\end{bmatrix} \tag{5}$$

$$\frac{Gm_1}{((x_3-x_1)^2+(y_3-y_1)^2+(z_3-z_1)^2)^{3/2}}\begin{bmatrix}x_1-x_3\\y_1-y_3\\z_1-z_3\end{bmatrix}+\frac{Gm_2}{((x_3-x_2)^2+(y_3-y_2)^2+(z_3-z_2)^2)^{3/2}}\begin{bmatrix}x_2-x_3\\y_2-y_3\\z_2-z_3\end{bmatrix}=\begin{bmatrix}\ddot{x_3}\\\ddot{y_3}\\\ddot{z_3}\end{bmatrix} \tag{6}$$

- Finite Differences
- Approximates the derivative
- Oldest
- Most straightforward

Central Finite Difference Coefficients

$$\begin{bmatrix} 1 & 1 & \dots & 1 & 1 \\ -p & -p+1 & \dots & p-1 & p \\ (-p)^2 & (-p+1)^2 & \dots & (p-1)^2 & p^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (-p)^{2p} & (-p+1)^{2p} & \dots & (p-1)^{2p} & p^{2p} \end{bmatrix} \begin{bmatrix} a_{-p} \\ a_{-p+1} \\ \vdots \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ m! \\ \vdots \\ 0 \end{bmatrix} \tag{7}$$

Ex. The 2-Body Problem

$$\frac{Gm_1 m_2}{r_{12}^2}\hat{r}_{12} = m_1 \ddot{\mathbf{r}}_1 \implies \frac{Gm_1 m_2}{r_{12,n}^2}\hat{r}_{12} = m_1 \frac{\mathbf{r}_1^{n-1} - 2\mathbf{r}_1^n + \mathbf{r}_1^{n+1}}{h^2} \tag{8}$$

Classical Mechanics - Computational Model

- Velocity Verlet Integration
- Useful for equations of motion
- Convserves energy
- The right choice for long time scales

Velocity Verlet

$$n = 0, 1, 2, 3, \ldots$$

$$\mathbf{r}_1^{n+1} = \mathbf{r}_1^n + \dot{\mathbf{r}}_1^n \Delta t + \frac{1}{2}\ddot{\mathbf{r}}\Delta t^2$$

$$\dot{\mathbf{r}}_1^{n+1} = \dot{\mathbf{r}}_1^n + \frac{\ddot{\mathbf{r}}_1^n + \ddot{\mathbf{r}}_1^{n+1}}{2}$$

Classical Mechanics - Computational Model

Algorithm 1: N-Body Gravitational Simulation

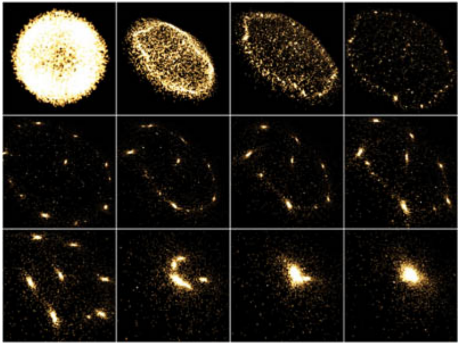
Input: Initial Positions, Initial Velocities, Masses

Output: The trajectory of the objects

```
Discretize the equations of motion
Use intial values r^0 and ṙ^0 to get r^1 through somthing like Euler integration
while t^n < t^f do
    for i ≤ N do
        Use discretized equation of motion for object i to get acceleration r̈_i^n
        Use Velocity Verlet to get new velocity ṙ_i^{n+1} and position r_i^{n+1}
    end
end
```

Classical Mechanics - Computational Model

- Forces can be calculated in parallel
- N-Body simulations can benefit from CUDA implementations[31]
- "50 times as fast as a highly tuned serial implementation (Elsen et al. 2006)"
- "250 times faster than our portable C implementation"



"Frames from an Interactive 3D Rendering of a 16,384-Body System..."

Classical Mechanics - Numerical Analysis

- Discretization Error
- Time step Δt
- Verlet error $= \mathcal{O}(\Delta t^2)$
- $\Delta t \rightarrow \Delta t/2 \implies$ error $\rightarrow$ error$/4$
- Verify results with energy conservation and energy drift

Electromagnetism

Electromagnetism - Mathematical Model

In general, the dynamics of the electric and magnetic fields are described by Maxwell's Equations

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{\rho}{\epsilon_0} & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} & \nabla \times \mathbf{B} &= \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}. \end{aligned} \tag{9}$$

Electromagnetism - Mathematical Model

Expanded

$$\partial_x E_x(t,\mathbf{r}) + \partial_y E_y(t,\mathbf{r}) + \partial_z E_z(t,\mathbf{r}) = \frac{\rho}{\epsilon_0} \qquad \partial_x B_x(t,\mathbf{r}) + \partial_y B_y(t,\mathbf{r}) + \partial_z B_z(t,\mathbf{r}) = 0$$

$$\begin{bmatrix} \partial_y E_z - \partial_z E_y \\ \partial_z E_x - \partial_x E_z \\ \partial_x E_y - \partial_y E_x \end{bmatrix} = -\partial_t \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix} \qquad \begin{bmatrix} \partial_y B_z - \partial_z B_y \\ \partial_z B_x - \partial_x B_z \\ \partial_x B_y - \partial_y B_x \end{bmatrix} = \mu_0 \rho \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} + \mu_0 \epsilon_0 \partial_t \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \tag{10}$$

as a coupled system of eight *partial* differential equations

Electromagnetism - Computational Model

- Finite Differences $\rightarrow$ Finite-Difference time-domain (Yee's Method)
- Multiple spatial dimensions $\implies$ discretized spatial mesh
- Also in time $\implies$ multiple runs over mesh computing gradients

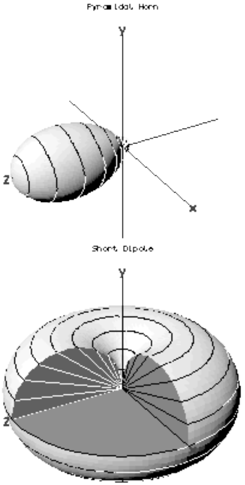


Figure: Antenna radiation pattern

Electromagnetism - Computational Model

Algorithm 2: Electromagnetism Evolution

Input: Initial State of the electromagnetic field

Output: Final state of the electromagnetic field

```
Discretize space into mesh
Discretize time into temporal chunks
for t_n < t_f do
    foreach cell in mesh do
        Calculate spatial derivatives
        Combine derivatives via Maxwell's Equations
        Get the electric and magnetic field
    end
    Calculate the time derivative of the whole mesh
end
```

Electromagnetism - Numerical Analysis

CFL Condition

Information in the simulation cannot travel faster than it would in reality.

- Rigorously,

$$\frac{\partial w}{\partial t} = u\frac{\partial w}{\partial x} \implies C = \frac{u\Delta t}{\Delta x} \leq C_{\text{max}} \tag{11}$$

- For explicit (time-marching) algorithms, $C_{\text{max}} = 1$.
- C_{max} is called the *Courant Number*.
- If the CFL condition is not met, the results are unphysical.

Quantum Mechanics

Quantum Mechanics - Mathematical Model

The Schrödinger equation is the quantum equation of motion

$$H\psi = E\psi \tag{12}$$

and for atoms and molecules

$$H = -\underbrace{\sum_i \frac{\hbar}{2m_e}\nabla_i^2}_{\text{e motion}} - \underbrace{\sum_k \frac{\hbar}{2m_e}\nabla_k^2}_{\text{Z motion}} - \underbrace{\sum_{i,k} \frac{e^2 Z_k}{r_{ik}}}_{\text{e-Z interaction}} + \underbrace{\sum_{i<k} \frac{e^2}{r_{ik}}}_{\text{e-e interaction}} + \underbrace{\sum_{k<l} \frac{e^2 Z_k Z_l}{r_{kl}}}_{\text{Z-Z interaction}} \tag{13}$$

Quantum Mechanics - Computational Model

- Molecular Mechanics $\rightarrow$ classical n-body simulation
- ab-initio Self-Consistent Field theory $\rightarrow$ iteratively solve the Schrödinger equation

Relativity

Relativity - Mathematical Model

The Einstein Field Equations

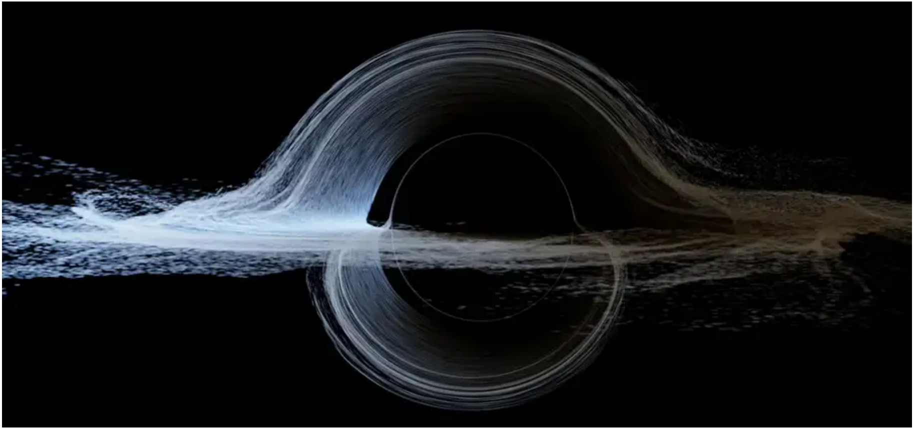
$$\underbrace{G_{\mu\nu}}_{\text{Curvature of Spacetime}} + \underbrace{\Lambda g_{\mu\nu}}_{\text{Expanding Spacetime}} = \kappa \underbrace{T_{\mu\nu}}_{\text{Mass and Energy}} \tag{14}$$

Actually 10 highly nonlinear, coupled partial differential equations in 4 dimensions.

Relativity - Computational Model

- OpenRelativity visualization[26]
- The physical scenarios considered, such as binary black hole mergers[35] and ray tracing near a black hole[23], yield forms of the EFEs that must be numerically solved with high-performance computing[27, 3, 14].

Relativity - Results



Conclusion

- All physics can use computers
- Even the simplest models need computation
- More complex mathematical models require high-performance computing
- Numerical analysis is of the utmost important when developing computational models and results

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