Octopus: Multisystem Example

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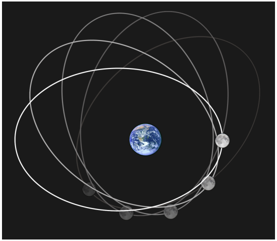
Testing the framework: celestial dynamics



- System of planets and moons as point particles interacting with gravity
- Numerical integration of orbits with different algorithms
- Easy to validate results
- Fast turnover for code development

Testing the framework: the velocity Verlet propagator

1. Update positions

$$\boldsymbol{x}(t+\Delta t) = \boldsymbol{x}(t) + \boldsymbol{v}(t)\Delta t + \frac{1}{2}\boldsymbol{a}(t)\Delta t^2$$

2. Update interactions with all partners (compute $\boldsymbol{F}(\boldsymbol{x}(t+\Delta t))$)
3. Compute acceleration $\boldsymbol{a}(t+\Delta t)$
4. Compute velocity

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \frac{1}{2}(\boldsymbol{a}(t) + \boldsymbol{a}(t+\Delta t))\Delta t$$

Testing the framework: the velocity Verlet propagator

```
! ------------------------------------------------------------
function propagator_verlet_constructor(dt) result(this)
  FLOAT,                        intent(in) :: dt
  type(propagator_verlet_t), pointer    :: this

  PUSH_SUB(propagator_verlet_constructor)

  SAFE_ALLOCATE(this)

  this%start_step = OP_VERLET_START
  this%final_step = OP_VERLET_FINISH

  call this%add_operation(OP_VERLET_UPDATE_POS)
  call this%add_operation(OP_UPDATE_INTERACTIONS)
  call this%add_operation(OP_VERLET_COMPUTE_ACC)
  call this%add_operation(OP_VERLET_COMPUTE_VEL)
  call this%add_operation(OP_STEP_DONE)
  call this%add_operation(OP_REWIND_ALGORITHM)

  ! Verlet has only one algorithmic step
  this%algo_steps = 1

  this%dt = dt

  POP_SUB(propagator_verlet_constructor)
end function propagator_verlet_constructor
```

Testing the framework: the velocity Verlet propagator

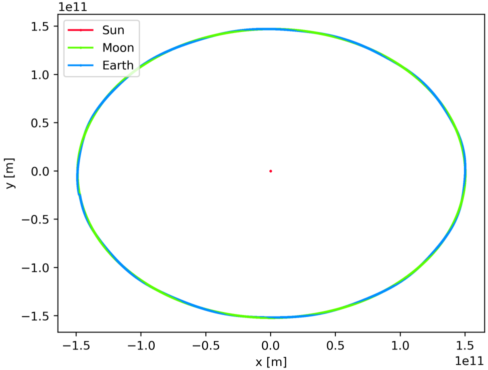
```
logical function classical_particles_do_algorithmic_operation(this, operation, updated_qu
  class(classical_particles_t),     intent(inout) :: this
  class(algorithmic_operation_t),   intent(in)    :: operation
  integer, allocatable,             intent(out)   :: updated_quantities(:)
  ...
  select case (operation%id)
  case (VERLET_START)
    if (.not. this%prop_data%initialized) then
      call this%prop_data%initialize(prop, this%space%dim, this%np)
      do ip = 1, this%np
        if (this%fixed(ip)) then
          this%prop_data%acc(:, ip) = M_ZERO
        else
          this%prop_data%acc(:, ip) = this%tot_force(:, ip) / this%mass(ip)
        end if
      end do
    end if
  case (VERLET_FINISH, BEEMAN_FINISH)
    call this%prop_data%end()
  case (VERLET_UPDATE_POS)
    this%pos(:, 1:this%np) = this%pos(:, 1:this%np) + prop%dt * this%vel(:, 1:this%np) &
      + M_HALF * prop%dt**2 * this%prop_data%acc(:, 1:this%np)
    updated_quantities = [POSITION]
```

Testing the framework: a simple case

Input

```
# List of systems to simulate, giving each one a name and declaring what type of system it is
%Systems  # (I am a block. Each line can have multiple columns. Columns are separated by a vertical bar)
 "Sun"   | classical_particle
 "Earth" | classical_particle
 "Moon"  | classical_particle
%

# Each system will interact through gravity with all possible partners
%Interactions
 gravity | all_partners
%

# We use velocitiy verlet for all systems
TDSystemPropagator = verlet

# Time step and total simulation time
TDTimeStep = 3600  # one hour
TDPropagationTime = 3*24*3600  # three days

# Next come the initial conditions, masses, etc
...
```

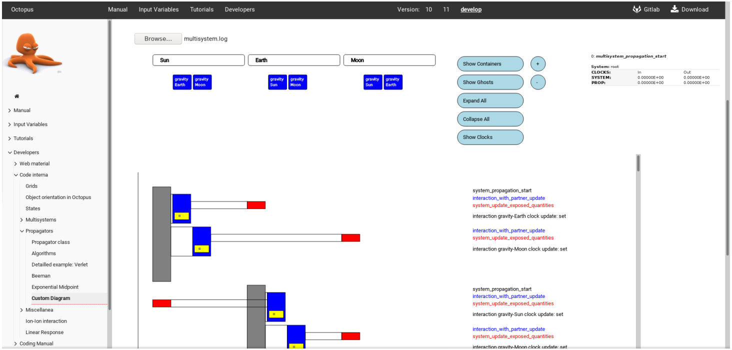
Testing the framework: a simple case



But how does this work in practice?

Visualizing the multi-system time-stepping algorithm

https://octopus-code.org/documentation/main/developers/code_documentation/propagators/custom_diagram/



Testing the framework: different time-steps

Input

```
# List of systems to simulate, giving each one a name and declaring what type of system it is
%Systems
 "Sun"   | classical_particle
 "Earth" | classical_particle
 "Moon"  | classical_particle
%

# Each system will interact through gravity with all possible partners
%Interactions
 gravity | all_partners
%

# We use velocitiy verlet for all systems
TDSystemPropagator = verlet

# Time step and total simulation time
Sun.TDTimeStep   = 3600   # one hour
Earth.TDTimeStep = 3600/2 # 30 minutes
Moon.TDTimeStep  = 3600/4 # 15 minutes
TDPropagationTime = 3*24*3600  # three days

# We need to allow for the interactions to use information that is behind in time
# Another way to handle this would be to use interpolation
InteractionTiming = timing_retarded

# Next come the initial conditions, masses, etc
...
```

Testing the framework: multi-systems and nesting

Input

```
# Top-level list of systems
%Systems
 "Sun"   | classical_particle
 "Earth" | multisystem   # This is a system of systems
%

# Here we specify the systems contained in the "Earth" system
%Earth.Systems
 "Terra" | classical_particle
 "Luna"  | classical_particle
%

# Each system will interact through gravity with all possible partners
%Interactions
 gravity | all_partners
%

# We use velocitiy verlet for all systems
TDSystemPropagator = verlet

# Time step and total simulation time
TDTimeStep = 3600  # one hour

TDPropagationTime = 3*24*3600  # three days

# Next come the initial conditions, masses, etc
...
```

Testing the framework: different algorithms

Input

```
# Top-level list of systems
%Systems
 "Sun"   | classical_particle
 "Earth" | multisystem   # This is a system of systems
%

# Here we specify the systems contained in the "Earth" system
%Earth.Systems
 "Terra" | classical_particle
 "Luna"  | classical_particle
%

# Each system will interact through gravity with all possible partners
%Interactions
 gravity | all_partners
%

# Use exponential-midpoint for Sun (NB: this propagator requires the evaluation of the forces at dt/2 and at dt
Sun.TDSystemPropagator = exp_mid_2step
Earth.TDSystemPropagator = verlet

# Time step and total simulation time
Sum.TDTimeStep   = 3600   # one hour
Earth.TDTimeStep = 3600/2 # 30 minutes

TDPropagationTime = 3*24*3600  # three days
```

Classical dynamics class diagram