Computing in Civil Engineering

AND GEOGRAPHIC INFORMATION SYSTEMS SYMPOSIUM

Proceedings of the Eighth Conference held in conjunction with A/E/C Systems '92

sponsored by the Technical Council on Computer Practices of the American Society of Civil Engineers

Hyatt Regency Dallas Hotel Dallas, Texas June 7-9, 1992

Edited by Barry J. Goodno and Jeff A. Wright

Published by the American Society of Civil Engineers 345 East 47th Street New York, New York 10017-2390

Two Paradigms for OOP Models for Scientific Applications

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This paper summarizes an alternative approach using declarative programming methods for the object oriented implementation of numerical codes. The alternative approach is illustrated through a comparison to an approach using the procedural language C++. The paper provides two separate OOP examples: (i) one making use of C++ and its message passing capabilities within an object framework, and (ii) one example which replaces message passing with simple assertions of and requests for object states.

Introduction

Object oriented programming (OOP) is quite promising as a representational tool for large scale scientific code development. Previous research efforts [Peeling, et. al., 1988; Angus and Thompson, 1989; Pearlman, et. al., 1990; Filho and Devloo, 1991; Ross, et. al., 1991] have discussed the use of object oriented programming (OOP) methods in the development and use of such codes. Implicit in these works was the desire to create an OOP environment where user code is easily modifiable and maintainable, where large-scale scientific user code is portable across a variety of architectures, and where the solution process is efficient when compared to serial, vector, or parallel FORTRAN environments. The key to effective OOP implementation in any environment is to create a representative object oriented design of the physical problem and its mathematical abstraction in the first place. This design places a premium on understanding the physical problem from the perspective of class structure, inheritance, and communication.

Constructing object based models requires knowledge of the structure and behavior of the objects in the system and of the interactions between the objects. Many OOP approaches provide constructs which allow for declarative descriptions of object structure, but they insist that the programmer model object behavior and interactions with a procedural "message passing" paradigm. Although procedural descriptions are useful where the intent is to model processes, it may be more natural to describe object system dynamics through declarations of the governing laws.

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The C++ Paradigm

C++ is not a pure object oriented language. One of the key design goals of the language can be stated as "you do not have to pay in storage or CPU time for what you do not use." Most OOP languages were designed with the overriding goal of mirroring a clean object oriented paradigm, without regard for efficiency at the language design level. Programs pay an efficiency penalty for this.

A more fundamental example of the difference between a pure OOP language and C++ is the inability to inline expand small functions. Consider the problem of adding two matrices (C=A+B). Operator + on matrices is a function call, which itself makes calls to operator [] on matrices (returning a vector) and operator + on vectors. The vector object has a similarly defined operator + and operator []. Also, operator = adds a matrix to a matrix and operator += adds a matrix to a vector. The addition of the keyword inline in front of a function call for very little actual code. Adding the keyword inline on a matrix adds no function call. Whether or not a message is a function call or inline expanded has no effect on the semantics of calling that message. This eliminates function call overhead since objects are not large functions.

Another feature of C++ is that default name resolution is static, which is to say that objects and messages between them are bound at compile time. In a pure OOP language, messages and objects are bound at run-time. Therefore, by passing many objects as parameters involved in the OOP paradigm. As long as name resolution is dynamic, which is to say binding is done OOP, and C++ does not allow this, after a fashion. By declaring a class or function to be "virtual", the user is directing the program to figure out the relevant typing information at run-time.

The behavior of physical phenomena is governed by a collection of clearly defined laws. Scientists normally describe these laws in the form of facts and rules, which contain references to the objects/dimension/ies of interest. But more often than not, as the scientist sets out to construct a theory/model, these declarative descriptions are necessarily translated into procedures with an associated loss in semantics accompanying the translation.

OOP helps reduce the disparity between the reality model and the information system model by providing the scientist with constructs which allow for a declarative description of object structure. But popular OOP languages (C++, Smalltalk, etc.) nevertheless insist that the scientist describe object behavior and interactions in terms of a procedural "message passing" paradigm. An extension to OOP which allows the scientist to describe object-system dynamics, behaviors of, and interactions between, objects using straightforward declarations of the governing physical facts and rules, could significantly minimize the time and effort required to create computer-based models, as well as improve the accuracy of simulations based upon these models.
An Example

The problem of one-dimensional heat conduction along a rod involves a partial differential equation relating the change in temperature, \( T \), to position, \( x \), along the bar as a function of time, \( t \), and the coefficient of thermal diffusivity, \( k \). The governing equation is of the parabolic form and is given here:

\[
\frac{\partial T}{\partial t} = \frac{k}{\alpha} \frac{\partial^2 T}{\partial x^2}
\]

The figures below illustrate the aggregation hierarchies (Figure 1) and the inheritance hierarchies (Figure 2) of the object structure for this simple problem. Each individual node in the discretized model is an object, as would the rod itself. The node object has three attributes and one of them, the node type, has two more. The node object has three attributes, length, material, and rod nodes. Material is represented by three attributes, length, material, and rod nodes. The material's representation in this problem actually models the parameter \( k \), but could include general attributes. The aggregation paths are represented by "has" in the properties for other problems. The aggregation paths in Figure 1 are shown as arrows with the same number or names in the form of arrows in Figure 1. There are as many rod nodes as there are nodes in the discretization of the rod. Figure 2 shows the paths of inheritance with "isa" arrows. Note that rod node inherits properties of the objects node and rod. For this particular problem rod node has a specific attribute associated with an Eulerian node type.

Figure 1. Aggregation Hierarchies

Figure 2. Inheritance Hierarchies

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What is interesting about the inner workings of this procedural example is that the explicit solver knows nothing about boundary conditions. It is a simple recursion of the form,

\[
T_{i,t} = T_{i-1,t} + \lambda (T_{i+1,t} - 2T_{i,t} + T_{i-1,t})
\]

for each spatial coordinate along the rod \( i \), and each time \( t \), and where \( \lambda \) is the stability number of the problem.

The solver is written to treat all rod nodes as internal. A C++ user code could be written, for example, to heat a rod in the middle, and observe how the temperature radiates outward. The user code would apply a method to the center rod node rather than to the ends, and initialize this rod node to the value of the heat source with the other rod nodes initialized to background. The governing equation (and the explicit solver embedded therein) would be left unchanged.

The implementation of the recursion in C++ is by passing messages to the associated rod node's temperature attribute to change the temperature at the rod node according to the formula. The temperature attribute in turn passes a message to the rod node. If a rod node is a temperature boundary node, it simply ignores the message. While boundary conditions are not difficult to model in 1D, many 2D and 3D problems have more complicated geometries on the boundaries. In this object-oriented system, the discrete solver is simply written as if all rod nodes were on the interior, and the boundary nodes modify the operation or cancel the operation themselves as necessary.

The user never needs to refer to the parameters \( \lambda \) or \( \Delta t \), the increment of each time step. The governing equation knows to set

\[
\Delta t = \frac{\lambda \Delta x^2}{k}
\]

where \( \lambda \) = stability constant and \( k \) = largest \( k \) in any node.

The solver knows the values of \( \lambda \) and \( k \) from querying the rod node's location and material attributes. The stability constant, \( \lambda \), can be changed by the user, but \( \lambda \) can have a default value. If the user is interested in the rate of convergence, the time step object is queried and a step method is used which applies the solver for one time step. In this one-dimensional example, all nodes are of the same material, but if there was a rod made of two or more materials, the material with the largest coefficient of thermal diffusion would determine the time step for solving the problem. If the user is interested in the steady state temperature distribution, he/she would use a converge object on the solver, which applies the solver at each time step and checks to see if the temperature at any rod node has changed by more than a user-prescribed tolerance. When this condition is no longer met, the method on the converge object will halt.

The Alternative Paradigm

This section contains a discussion of possible extensions to OOP which could appreciably limit the number of declarative-to-procedural translations required by many OOP languages. Additionally, these extensions provide for the encapsulation of an object's behavioral properties along with its structural properties, thereby increasing the ease with which the object may be reused in related applications. This section also demonstrates how conventional message passing can be replaced with
simple assertions of and requests for object states. This would simplify the user interface to something similar to that found in conventional data-base systems. Our "Alternative Paradigm" is largely derived from the ontological approach for evaluating system design/analysis methodologies described by Wand and Weber (1980). We substitute the word "object" in this paper for the word "thing" used by Wand and Weber. The following points provide a quick overview of the pertinent aspects of the ontological mindset:

- The world is comprised of objects having properties (attributes).
- An object may contain other objects (that is, each object need not be atomic).
- Objects may be organized into an object system (a set of objects).
- An object is modelled in terms of a functional schema (a set of functions), where each function assigns a value to an attribute at a given time.
- The collection of every attribute's value(s) comprises the state of the object (a perceptible change to an object occurred only if its state changed).
- A change in the state of an object is termed an event.
- There are two types of events: external, where another object has asserted a new state for the object and, internal, where the object has changed its own state through the application of its stability laws.

- An object's stability laws define its stable states and its response to those external events which request that the object assume an unstable state.

We augment the ontological approach with a formal treatment of time, similar to that in the ontological model discussed by Langitris (1980). In this treatment an object assumes a particular state at a particular time.

Our extension primarily employs a hybrid of the ontological and infological models, where a programming task may be decomposed into three functions: 1) using declarations of the governing facts and rules, describe all pertinent object system structure and behavior, 2) identify external events (changes in the state of one or more objects), and 3) pose queries against the system.

Structure and Behavior of the Object System

We describe object structure using conventional inheritance ("isa") and aggregation ("has") hierarchies. Object behavior is described using a rule-based syntax (similar to traditional expert-systems) where each rule's head identifies an unstable state, and each rule's body maps the unstable state onto a stable state, i.e.,

```star
* object structure *
  window isa object which has size, location, and color,
  window.size has width and height,
  window.1st_left isa integer.
  ...
  window.location.top_left and bottom_right,
  window.location.top_left has row and column.
  window.location.top_left.row isa integer.

* object behavior *
  if window.location.top_left < 0 then window.location.top_left = 0.
  ...
  window.location.bottom_right = window.location.top_right - window.size.height.
```

Note that this model makes no distinction between an object and its class. If window has yellow color and square shape, and window-1 is a window, then window-1 also has yellow color and square shape.

An Example

Suppose we wanted to examine the one-dimensional heat conduction along a road, as discussed earlier. The object system (itself an object) is the road. The description of the road would contain stability rules and facts which define the heat conduction along the road among the road_nodes. In this example, the stability rules would be comprised of the explicit solver, which is used to determine the state of the internal road_nodes. We augment the definition of node with the rule,

```star
If node.type = Faberan
  Then node.temp(time=t+1 and location=i) =
    node.temp(time=t and location=i) +
    (1/node.temp(time=t and location=i) +
    2*node.temp(time=t and location=i))
    node.temp(time=t and location=i+1))
```

The scientist initializes the system by specifying the initial and boundary conditions, by asserting values for temperature and location attributes of each road_node. So, if the external boundary conditions were temp=-100°C and temp=50°C at the left end and right end of the road, respectively, and the internal nodes were set to some ambient temperature, say temp=0°C, then following facts would represent the state of the road,

```star
node.temp(time=0 and location=0) = 100
node.temp(time=0 and location=1) = 50
```

When the scientist queries the system for the state of a road_node at a new time, this places the object system in an unstable state. For example,

```star
node.temp(time=3 and location=1) =?
```

The object system then applies its stability rules to adjust each road_node until the object system is again stable, and returns the answer to the scientist's query. Alternately, the scientist can query for the time at which a road_node has a specific temperature, which again causes the object system to fire its stability rules. For example,

```star
node.temp(time=3 and location=1) =70.
```

Conclusions

This paper introduces two separate OOP paradigms for addressing scientific computations, one dealing with the language C++ and another called the "alternative" paradigm. The two paradigms are distinguished in terms of their design for OOP for the following items. The paper gives an example of programming with the alternative paradigm, and provides technical models using each of the paradigms.
In the conventional C++ approach, knowledge about the structure of an object is separated from the knowledge of its behavior; message passing specifies the behavior. A procedural language is used to explicitly code the physical laws. Each user code, although modular, has a specific structure associated with a specific physical application. Any changes to one area of the knowledge base can have an impact on other knowledge in the database.

For the alternative OOP paradigm, knowledge of the behavior of an object and knowledge of the structure of the object are both attributes of the object. A declarative language codes the knowledge of the physical laws as facts and rules so that they don't need to be translated into procedures, as is the case using a procedural language. The rules and physical laws are stored in the knowledge base and various applications are implemented as specific questions about the "state" of the object. State changes are handled by rules that specify how to transition from the unstable state back to a stable state. Changes to one area of the knowledge base have few or no effects on the rest of the knowledge base.

Although much remains to be done to make OOP a realistic and useful computational tool for scientists and engineers in their attempts to model the physical world, the few works developed in this field have shown tremendous potential.

References


