

POINT KINETICS*

CLYDE HUIBREGTSE†

Abstract. This is an example SIAM L^AT_EX article. This can be used as a template for new articles. Abstracts must be able to stand alone and so cannot contain citations to the paper’s references, equations, etc. An abstract must consist of a single paragraph and be concise. Because of online formatting, abstracts must appear as plain as possible. Any equations should be inline.

Key words. example, L^AT_EX

AMS subject classifications. 68Q25, 68R10, 68U05

1. Point Kinetics and Reactor Dynamics.

1.1. The Motivation for a Simpler Model. Reactor dynamics are governed by the transport of energetic neutrons throughout the active core. In particular, we define the diffusion of these neutrons in Eq. (1.1).

$$(1.1) \quad \frac{\partial N(\vec{r}, t)}{\partial t} = Dv\nabla^2 N - \Sigma_a v N + S$$

where $N(\vec{r}, t)$ and $S(\vec{r}, t)$ are the neutron density and produced additional neutron density in some volume dV at location \vec{r} at time t . D is the diffusion constant; v is the neutron speed; and Σ_a is the macroscopic neutron absorption cross-section. (CITE)

Note that this partial differential equation effectively encodes the conservation of neutrons throughout the core. Neutrons in a given volume of fuel can: (1) move to an adjacent volume, (2) be absorbed in the given volume, or (3) be generated as a result of a fission within the volume.

This branching structure lends itself wonderfully to the use of Monte Carlo codes to simulate neutron transport in very high fidelity (CITE SERPENT). Unfortunately, modeling macroscopic reactor behavior with these high fidelity tools is infeasible. Coupling the thermalhydraulic behavior of the plant’s power conversion system to the dynamics of subatomic neutrons is computationally intractable. Consequently, we must create an abstraction from the neutronics to core-wide dynamics that effectively model important plant behavior without knowledge of individual neutrons. To do this, we use the Point Reactor model.

1.2. The Point Reactor. The point reactor model operates under a few critical assumptions. First, it is assumed that the neutrons included in $N(\vec{r}, t)$ are all of a single energy (for our purposes, this is “fast”, rather than “thermal” energies). Additionally, our treatment of the neutron production term $S(\vec{r}, t)$ in Eq. (1.1) must be formally defined for the point reactor. As shown in Eq. (1.2), produced neutrons can be of two types: *prompt* and *delayed*. Prompt neutrons are produced through direct fission of fuel nuclei, while delayed neutrons are the byproduct of fission-product decay significantly later than the prompt generation.

*Submitted to the editors DATE.

†Massachusetts Institute of Technology Departments of Mathematics and Physics (huibregc@mit.edu, www.google.com).

$$(1.2) \quad S(\vec{r}, t) = \underbrace{(1 - \beta)k_{\infty}\Sigma_a v N}_{\text{prompt generation}} + \underbrace{\Sigma_i \lambda_i C_i}_{\text{delay generation}}$$

The proportionality constants shown in Eq. (1.2) are outside the scope of this analysis. However, C_i refers to the current concentration of “delayed neutron group” i . It has been shown that the inclusion of six delayed neutron groups constitutes a reasonably accurate approximation of reactor dynamics. (CITE FOR NEUTRON GROUPS - Keepin 1965)

The final, and most critical assumption the Point Reactor model makes can be defined as follows: (1) the densities of prompt and delay neutrons are separable in time and space, and (2) the spatial dependence of prompt neutron density matches that of delayed neutron density.

While the derivation of these final differential equations is outside the scope of this analysis, they are reproduced in Eqs. (1.3) and (1.4).

$$(1.3) \quad \frac{dn}{dt} = \frac{\rho - \beta}{\Lambda} n + \Sigma_i \lambda_i c_i$$

$$(1.4) \quad \frac{dc_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i c_i$$

Here, formal definition of the parameters is critical to understanding of the following analysis. Parameters are defined in Eqs. Equations (1.5)–(1.10).

(1.5) n = normalized number of neutrons in the core (effective reactor power)

(1.6) c_i = normalized number of delayed neutrons of group i

(1.7) ρ = external reactivity (pcm)

(1.8) β = delayed neutron fraction ($\Sigma_i \beta_i$)

(1.9) Λ = mean neutron generation time (s)

(1.10) λ_i = precursor time constants (1/s)

This ordinary differential equation (ODE) constitutes the primary focus of this analysis.

1.3. Important Concepts for this Analysis. In order to fully understand the process by which we examine this dynamical system, one must be acquainted with the following terms that are used to describe particular features of a reactor transient.

DEFINITION 1.1. *External Reactivity:* External reactivity is defined as an artificial addition (or subtraction) of some fraction of the total reactor neutron population. We call any external reactivity, an “insertion”, whether or not it has positive or negative value. It is measured in pcm, or per cent mille (0.001%)

DEFINITION 1.2. *Dollar (reactivity):* One dollar of reactivity (\$) is defined as the reactivity required to cross the threshold from delayed criticality to prompt criticality. It is numerically equal to the β constant defined in Eq. (1.8).

DEFINITION 1.3. *Prompt Criticality:* *Prompt criticality refers to a reactor state in which a positive feedback nuclear chain reaction is sustained entirely by the generation of prompt neutrons. This differs from delayed criticality in that it does not require the presense of delayed neutron groups to maintain its fission chain reaction. Prompt criticality is characterised by fast spikes in power due to the short generation times for prompt neutrons.*

1.4. Analytical Jacobian Analysis. The form of the ODE defined in Eqs. (1.3) and (1.4), lead to an analytical definition of this system's Jacobian. (CITE GANOPOL) Particularly, our system is as defined in Eq. (1.11), so there exists a true form of the Jacobian, shown in Eq. (1.12).

$$(1.11) \quad \frac{du}{dt} = A(t)u$$

$$(1.12) \quad A(t) = \begin{pmatrix} \frac{\rho(t)-\beta}{\Lambda} & \lambda_1 & \lambda_2 & \cdots & \lambda_6 \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & 0 & \cdots & 0 \\ \frac{\beta_2}{\Lambda} & 0 & -\lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\beta_6}{\Lambda} & 0 & 0 & \cdots & -\lambda_6 \end{pmatrix}$$

Here, $A(t)$ is the time dependent Jacobian for our dynamical system. Note the time independence for all but the prompt neutron term. This is a critical feature of the system. We can see that, at operating conditions where $0 \leq \rho(t) < \beta = 1\$, all of the diagonal terms of our Jacobian are negative. This property ensures that the reactor is in a delayed critical state, and the unbounded growth in power is relatively slow. Transients in which $\rho(t) \geq \beta = 1\$ have Jacobians with a positive diagonal element. This corresponds to the reactor going prompt critical, and the reactor power grows without bound millions of times faster than when it is delayed critical.$$

There are a few things to note: (1) the unbounded growth of reactor power seen in transients with positive $\rho(t)$ parameters is a numerical result. In reality, nuclear material undergoes a “fizzle” (CITE) that limits this rapid overpower (except in the cases of nuclear weapons). This effect is not captured in the Point Reactor model, but does not affect solutions around the time of reactivity insertion. (2) For sections of a reactor transient timeseries over which $\rho(t)$ is constant, there is an analytical solution to the dynamical system involving a series of exponential functions defined by the eigenvalues of A .

For the purposes of building a modeling tool that can aid in iterating reactor design, we focus our analysis on the efficacy of solver methods on the order of 100pcm reactivity insertions. These insertions correspond to moderate transients seen during normal operations.

1.5. The Analytical Solution to the Step Insertion. As previously stated, in cases where $\rho(t)$ is constant, there exists an analytical solution to the point kinetics ODE. This solution is reproduced in Eq. (1.13).

$$(1.13) \quad \Psi = \sum_{k=0}^K \left((-1)^k \sum_{j=0}^K \left(\frac{e^{\omega_j t} B_{K-k,j}}{\prod_{i=0, i \neq j}^K (\omega_i - \omega_j)} \right) A^k \right) \Psi_0$$

$$(1.14) \quad \text{where } B_{m,n} = \sum_{i_1=1, i_1 \neq j}^K \sum_{i_2=i_1+1, i_2 \neq j}^K \dots \sum_{i_m=i_{m-1}+1, i_m \neq j}^K \omega_{i_1} \omega_{i_2} \dots \omega_{i_m}$$

(CITE SOLUTION) Each ω_i is an eigenvalue of the Jacobian A , or is a root of the inhour equation:

$$(1.15) \quad \rho = \Lambda \omega + \omega \sum_{k=1}^K \frac{\beta_k}{\omega + \lambda_k}$$

This is the solution to which we compare all of our computed timeseries to give a metric for accuracy in this test case.

2. Solving the Point Kinetics Equations.

2.1. Building an Optimal Derivative Definition. In order to perform any sort of reasonable benchmarking for solver algorithms, we must ensure that our ODE definition is optimal, such that any discrepancies in solution time are not drowned out by overhead. There are a few things we can check to ensure optimality in our ODE definition: (1) memory allocations, (2) type stability, and (3) solver overhead.

The point kinetics module written for this analysis is reproduced below:

```

module point_kinetics
  abstract type AbstractInsert end
  # (p :: AbstractInsert)(t :: Float64) :: Float64

  struct StepInsert <: AbstractInsert
    r :: Float64
    t :: Float64
  end

  (insert :: StepInsert)(t :: Float64) :: Float64 = t > insert.t ? insert.r : 0.

  struct PKparams
    r :: AbstractInsert
    l :: Float64
    b :: Float64
    lams :: Array{Float64, 1}
    bets :: Array{Float64, 1}
  end

  function pk!(du, u, p, t)
    r = p.r
    l = p.l
    b = p.b
    lams = p.lams
    bets = p.bets
  end

```

```

158
159     prec_conc = @view u[2:end]
160     d_prec_conc = @view du[2:end]
161
162     du[1] = (r(t) - b)*u[1] / 1 + lams' * prec_conc
163
164     d_prec_conc .= bets .* u[1] ./ 1 .- lams .* prec_conc
165 end
166
167 export pk!, PKparams
168 end

```

Using the `BenchmarkTools.jl` `@btime` and `@benchmark` macros, we can demonstrate that our inner loop (the `pk!` method) has minimal allocations. Particularly, we can achieve almost no (12) heap allocations per inner loop, totalling only 256 bytes.

Now we can use the type inferencing capabilities of Julia's JIT compiler to speed up our solves. The `@code_warntype` macro shows no potential type ambiguities throughout our inner loop, so we can be assured the JIT compiler is producing optimal type inferences.

Finally, we can use the `Profile.jl` module to generate a Flame plot. This plot shows the relative time spent in each function called during the solve. Highlighted in Figure ?? are sections of importance. In general, though, there is little overhead from the solver, so most of the computation time is spent doing the actual integration.

Now we can effectively dive into a solver analysis with the guarantee that algorithmic differences in the integrators produce the variance in the total runtimes, and not computational inefficiencies.

2.2. Work-Precision Diagrams. In this section we present a detailed analysis of the efficacy of a litany of solvers at a variety of tolerances. The best metric for rating the performance of a solver algorithm is an open question. The best choice is user-specific, so for the sake of making a conclusion, we specify our user needs here. We set out to create a high-speed, reasonably accurate simulator to be used in core design work and reactor control optimizations. There are a few key threshold criteria that we require of our simulator:

1. Resolve neutron densities to an accuracy within 0.1
2. Have the ability to accept a reactivity insertion of arbitrary shape (not necessarily of arbitrary magnitude - mentioned during the discussion of prompt criticality)
3. Outperform an existing Python implementation.

Appendix A. An example appendix.

LEMMA A.1. *Test Lemma.*

Acknowledgments. We would like to acknowledge the assistance of volunteers in putting together this example manuscript and supplement.