



Theory-Software Translation: Research Challenges and Future Directions

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RESEARCH ARTICLE

The challenges of theory-software translation [version 1; peer review: awaiting peer review]

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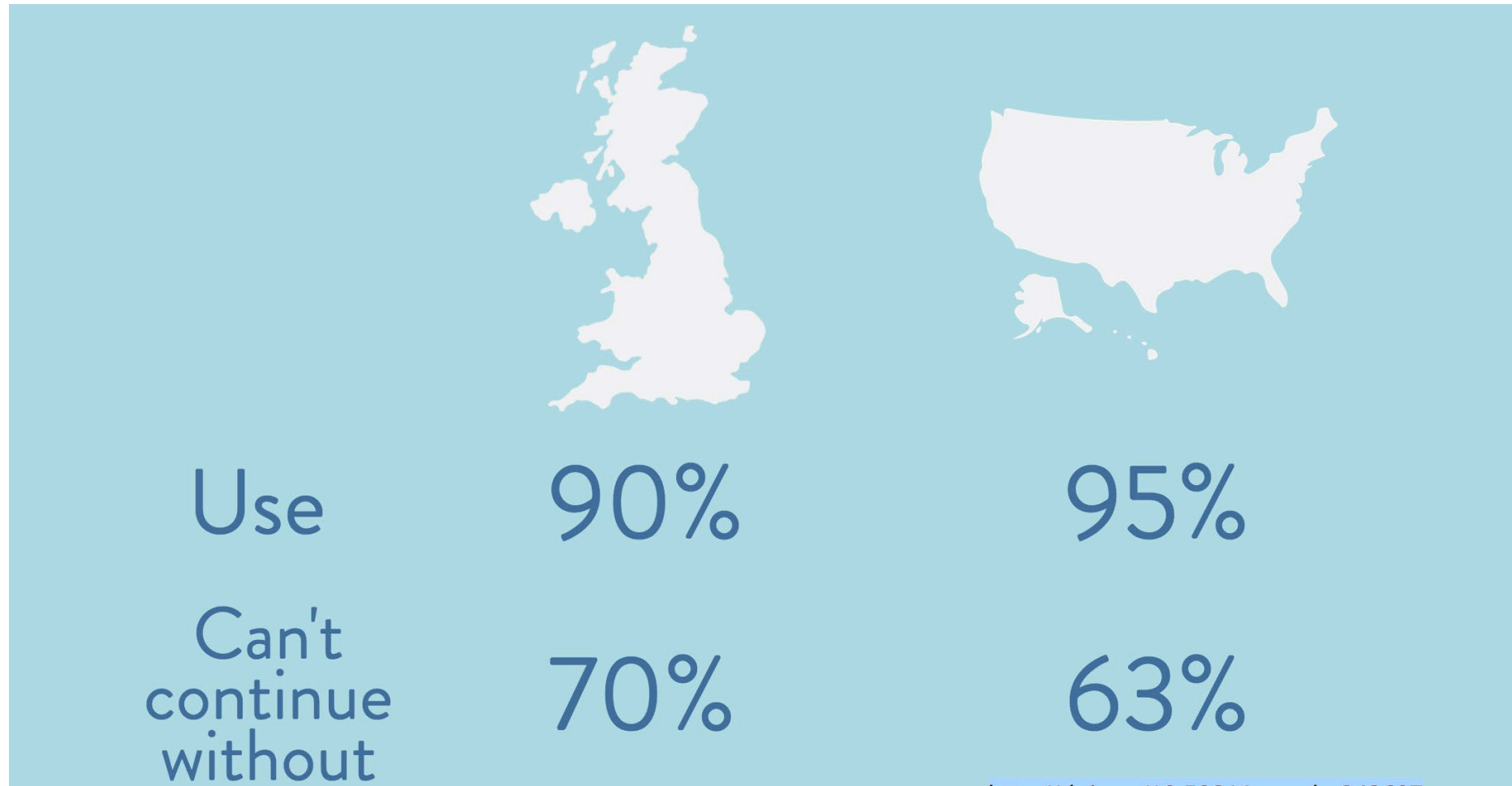
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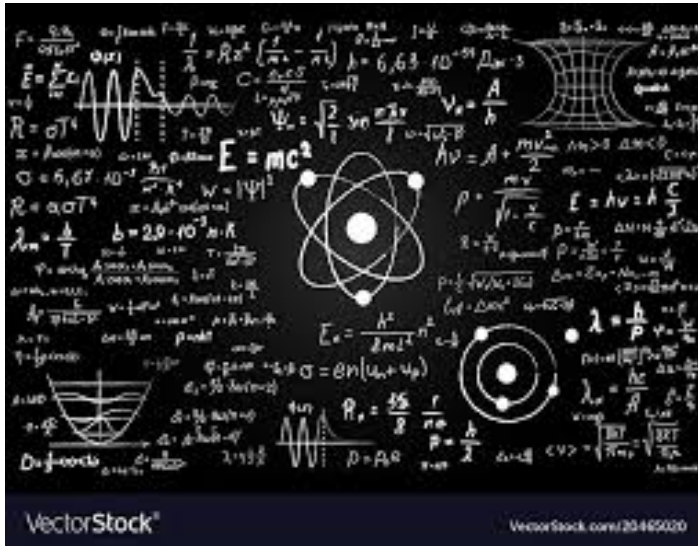
⁷Argonne National Laboratory, Argonne, USA

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Use of Software for Research



Theory-Software Translation



Translate



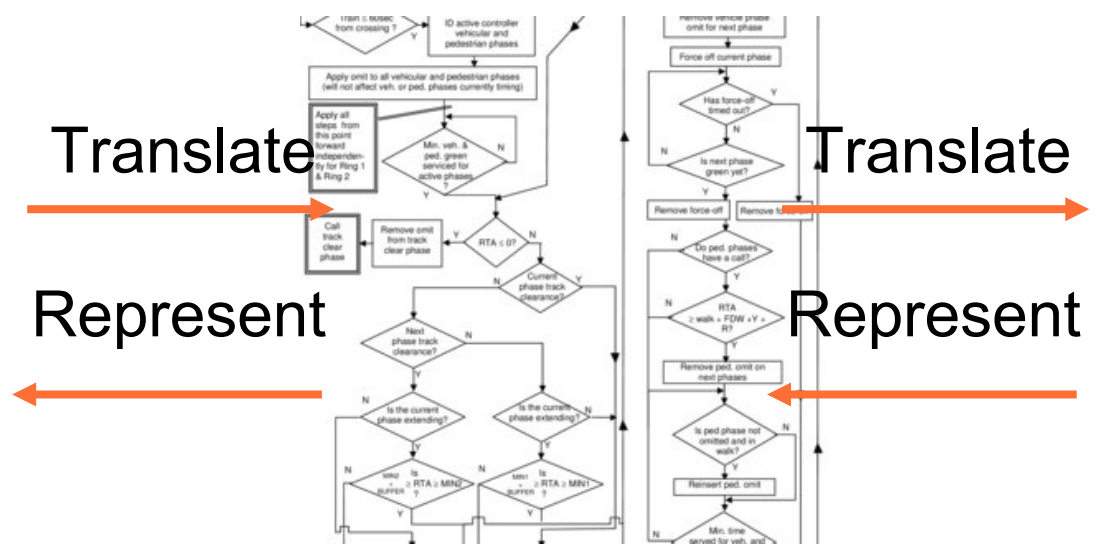
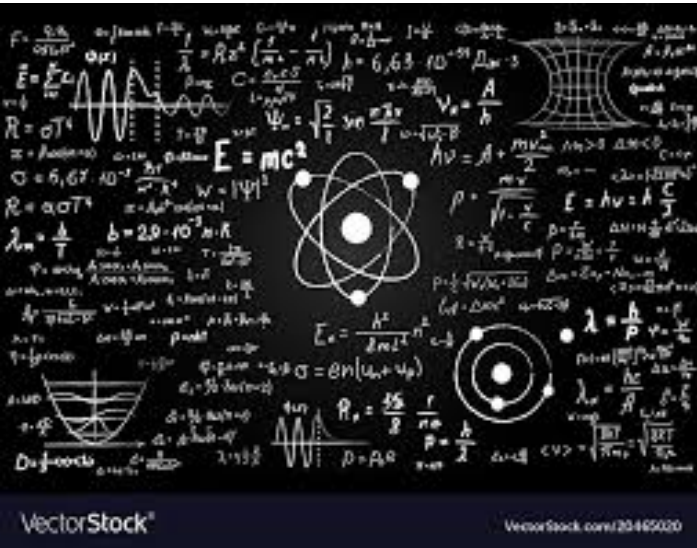
Represent



```

each: function(o, t, n) {
  var r, i = 0;
  n = o.length;
  n = N(n);
  if (n) {
    if (o) {
      for (i = 0; i < n; i++) {
        if (r = t.apply(o[i], n), r === !1) break;
      }
    } else {
      for (i in o) {
        if (r = t.apply(o[i], n), r === !1) break;
      }
    }
  } else if (o) {
    for (i = 0; i < n; i++) {
      if (r = t.call(o[i], i, o[i]), r === !1) break;
    }
  } else {
    for (i in o) {
      if (r = t.call(o[i], i, o[i]), r === !1) break;
    }
  }
  return o;
},
trim: b && !b.call("luffeffu0000") ? function(e) {
  return null == e ? "" : b.call(e);
} : function(e) {
  return null == e ? "" : (e + "").replace(C, "");
},
isArray: function(e, t) {
  var n = t || [];
  return null != e && !(Object(e)) ? x.merge(n, "string" == typeof e ? [e] : e) : b.call(n, e);
},
isArray: function(e, t, n) {
  var r;
  if (n) {
    if (n) return n.call(t, e, n);
    for (r = t.length, n = n ? Math.max(0, r + n) : 0; r > n; n++) {
      if (n in t && t[n] === a) return n;
    }
  }
}
    
```

Theory-Software Translation



Translate

Translate

Represent

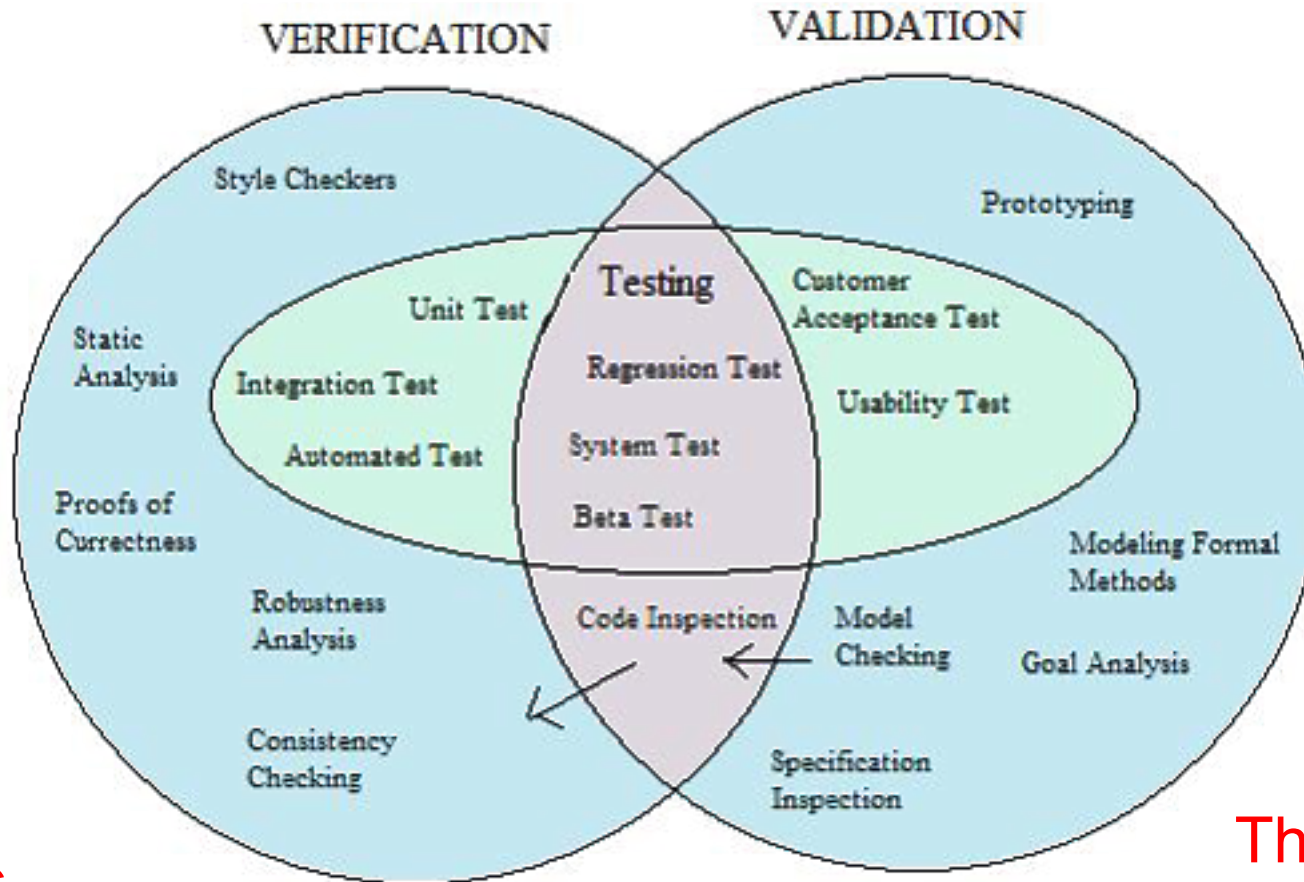
Represent

```

each: function(e, t, n) {
  var r, i = 0,
      o = e.length,
      s = n(t);
  if (n) {
    if (s) {
      for (; i < o; i++)
        if (r = t.apply(e[i], n), r === !1) break;
    } else if (s) {
      for (; i < o; i++)
        if (r = t.call(e[i], i, e[i]), r === !1) break;
    } else if (s) {
      for (; i < o; i++)
        if (r = t.call(e[i], i, e[i]), r === !1) break;
    }
    return e;
  },
  trim: function(e) {
    return null == e ? "" : e.call(e);
  },
  function(e) {
    return null == e ? "" : (e + "").replace(C, "");
  },
  isArray: function(e, t) {
    var n = t || [];
    return null != e && (Object(e)) ? x.merge(n, "string" == typeof e ? [e] : e) : e.call(n, e);
  },
  isArray: function(e, t, n) {
    var r;
    if (t) {
      if (n) return e.call(t, n);
      for (r = 0; r < e.length; r++)
        if (n(e[r], r, e)) return !0;
    }
    return !1;
  }
}

```

Verification and Validation - Challenges



Am I building the product right?

Am I building the right product?

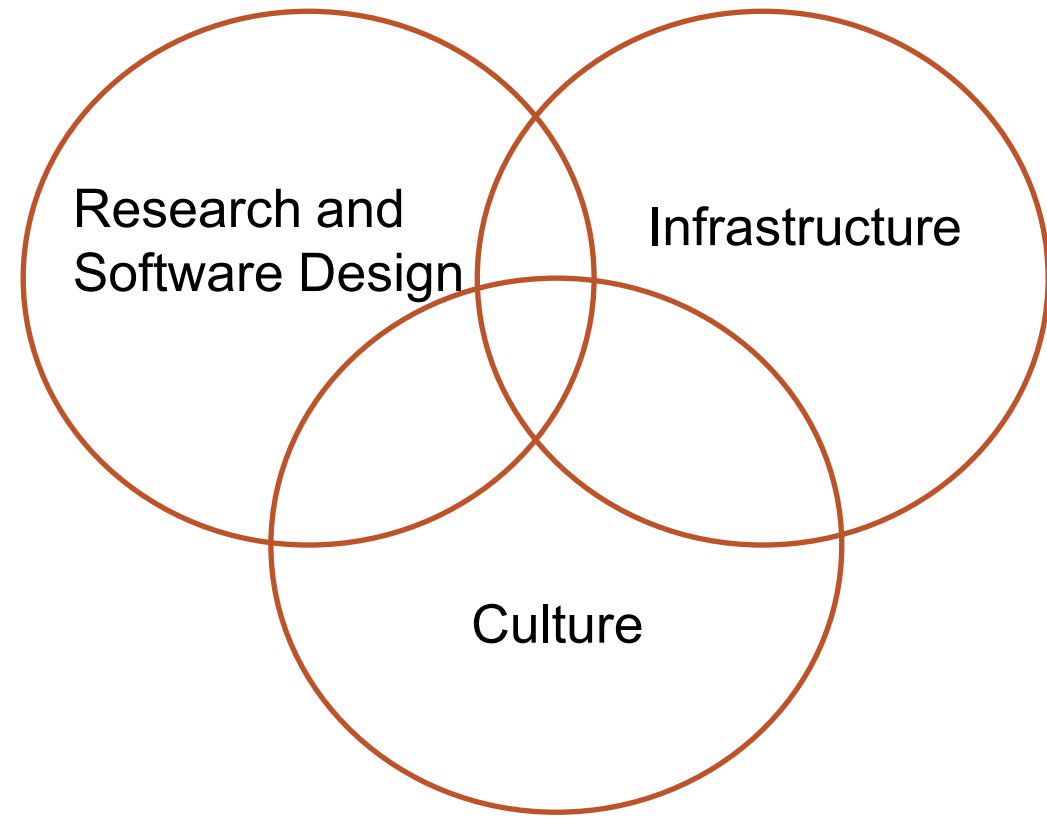
Error Sources

The science is wrong

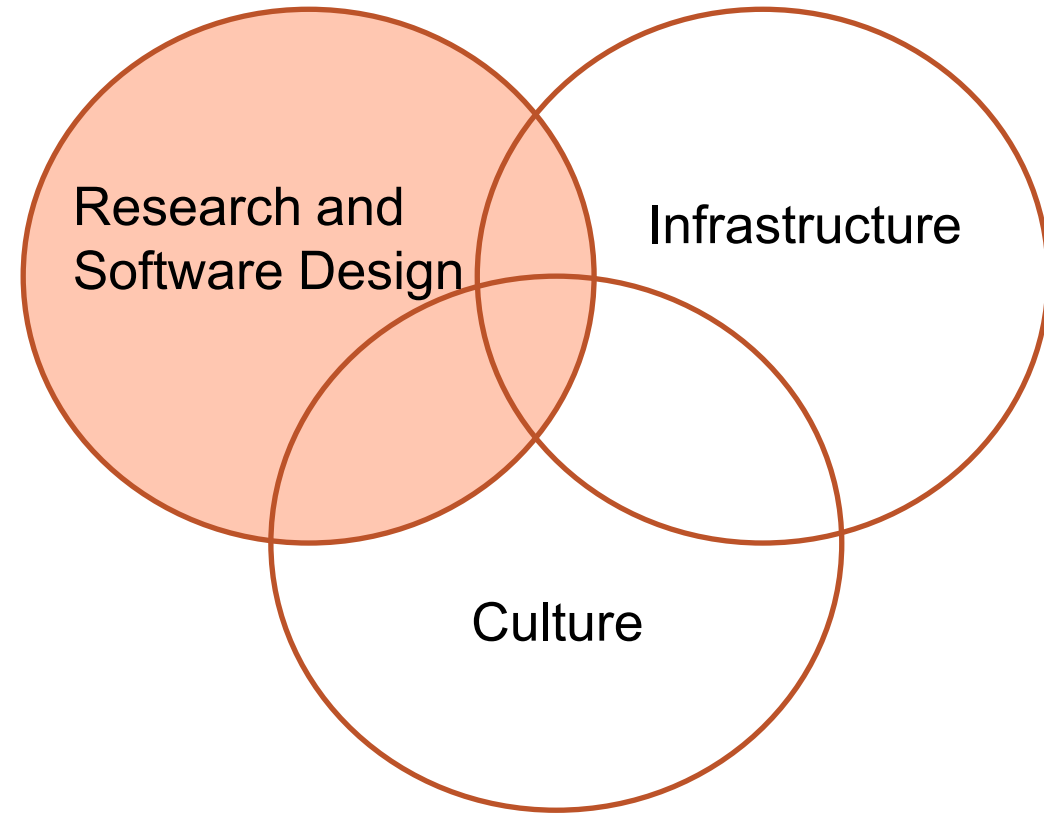
The software is wrong

The translation process incurs loss or ambiguity: mathematics presents “what is”, computational translation “how to”

Challenges in Three Areas

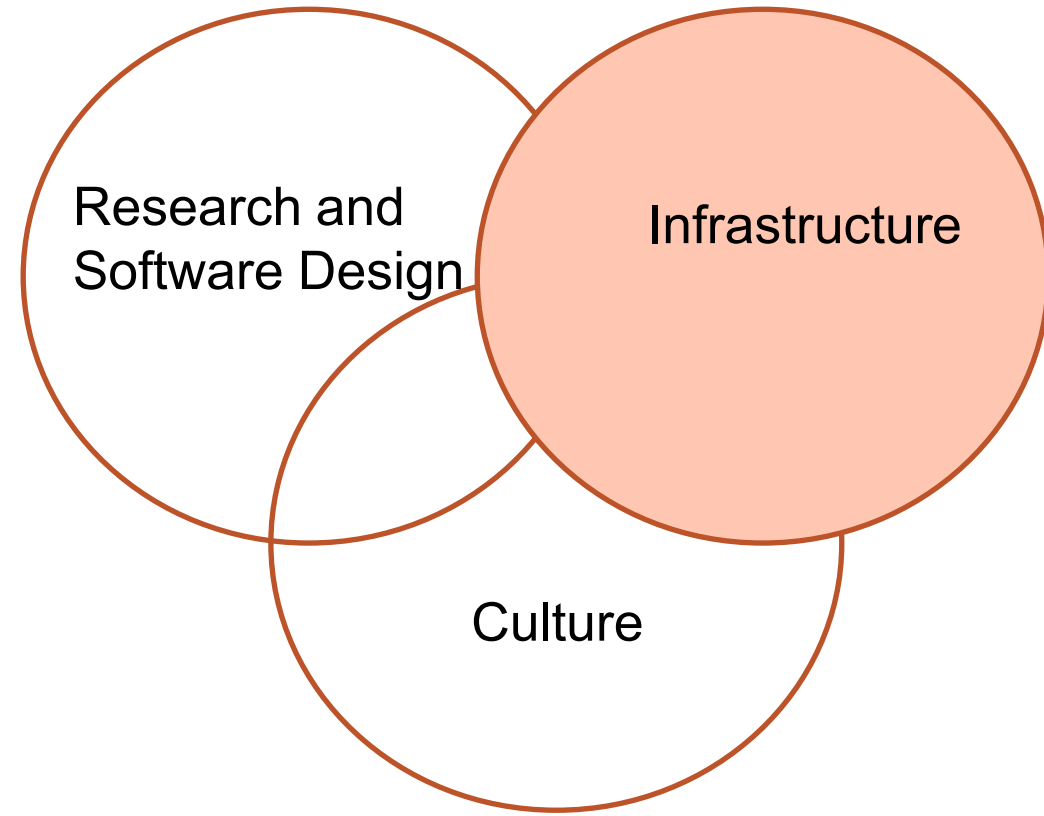


Emerging Topics in Research and Software Design



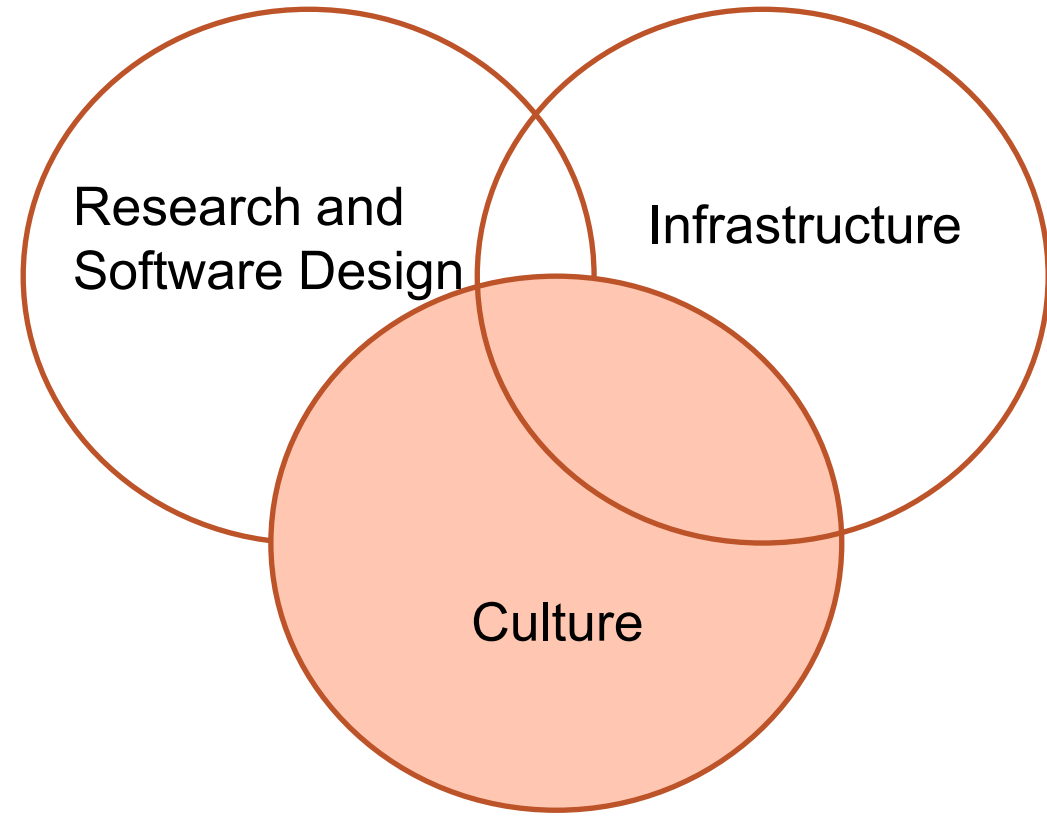
- Can/should we separate concerns?
- Should theory be readable from software?
- What are the effects of automation in programming?
- How can we evaluate the design process?
- How can we better link domain science and computer science?

Emerging Topics in Infrastructure



- How should we verify results arrived at through computation?
- How should we address reproducibility and sustainability?
- What are the constraints posed by platforms and architectures?
- Measuring uncertainty in theory-software translation

Emerging Topics in Culture



- How can we foster a culture of collaboration?
- What are the external expectations of the reliability of the software?
- How does the research environment affect the translation process?
- What is the best way to embed software engineering skills in science?

Thank you!

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