Chemistry Across Multiple Phases (CAMP): An integrated multi-phase chemistry model

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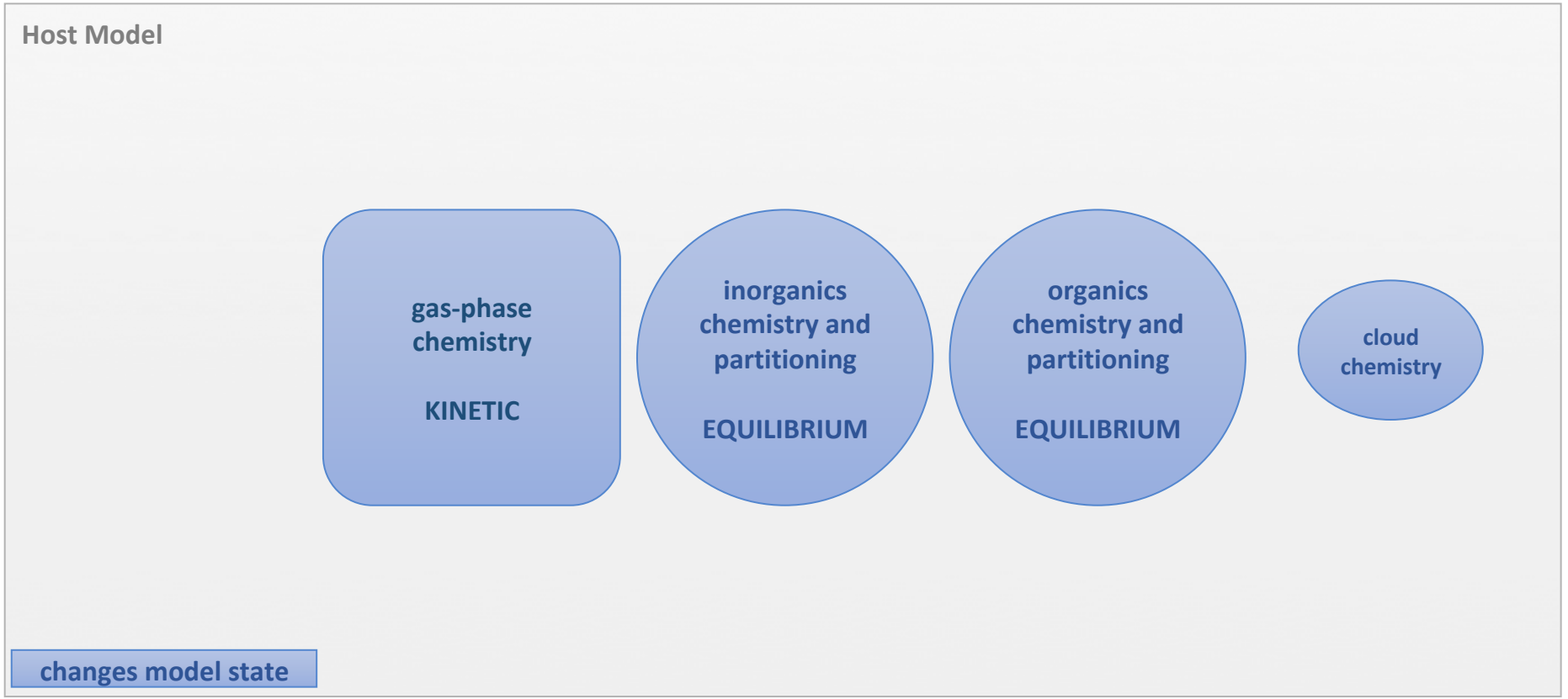
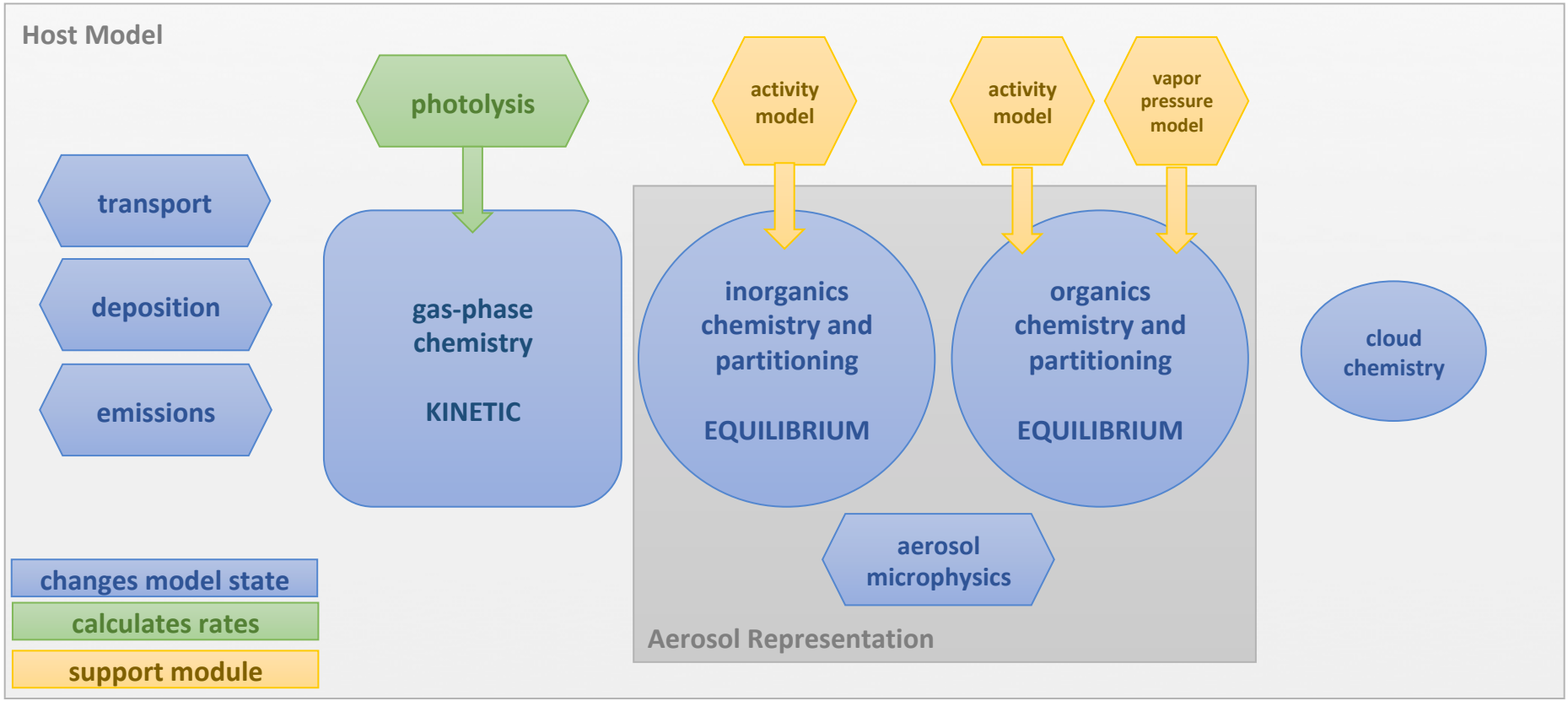
CESM Atmosphere & Whole Atmosphere & Chemistry-Climate WG Meeting

Motivation—Chemistry in Atmospheric Models



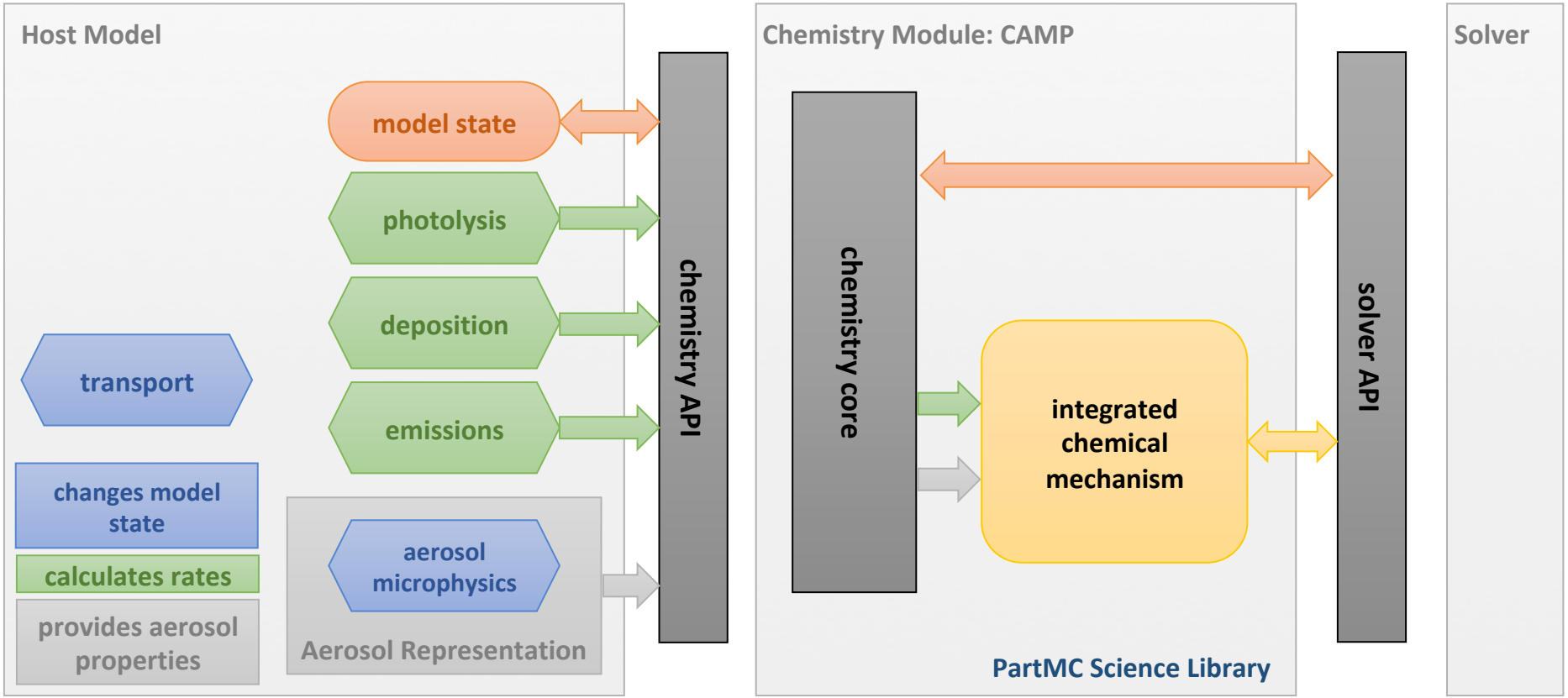
Motivation—Chemistry and Related Modules



Design Goals

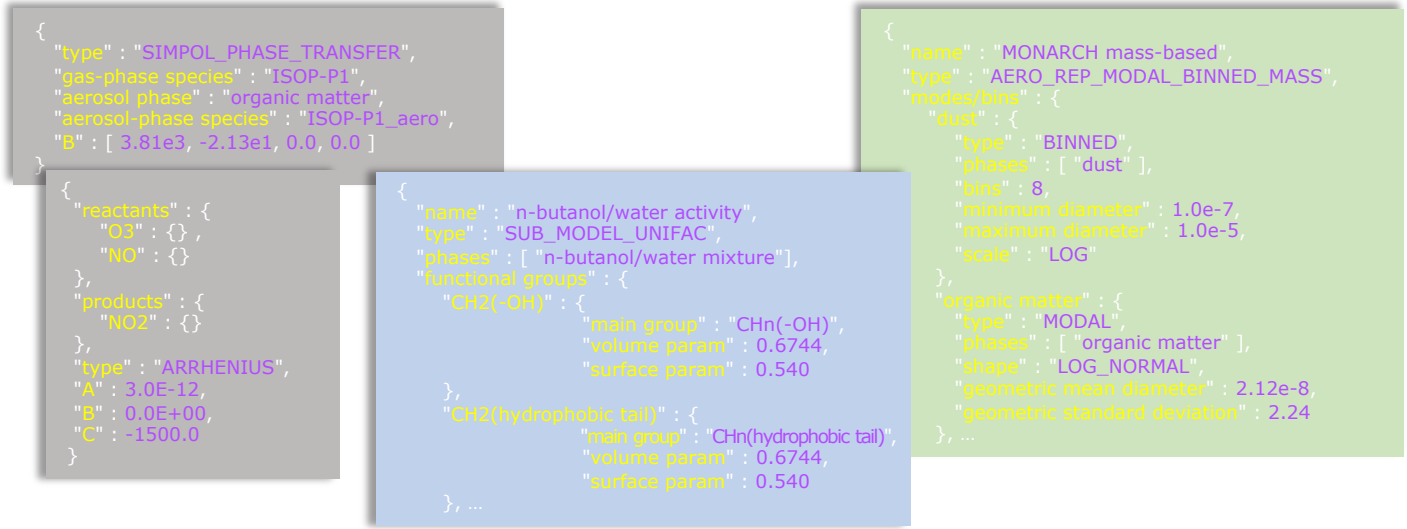
- **Treat chemistry, partitioning and related processes kinetically as one system to solve**
- **Make it flexible**
  - Usable by modelers and experimentalists
  - Portable between models (chamber, plume, regional, global)
  - Object oriented design
  - JSON configuration files
- **Make it efficient**
  - Scalable chemical complexity
  - Condensed data structure
  - Porting to GPUs

Approach—Integrated Chemistry Module

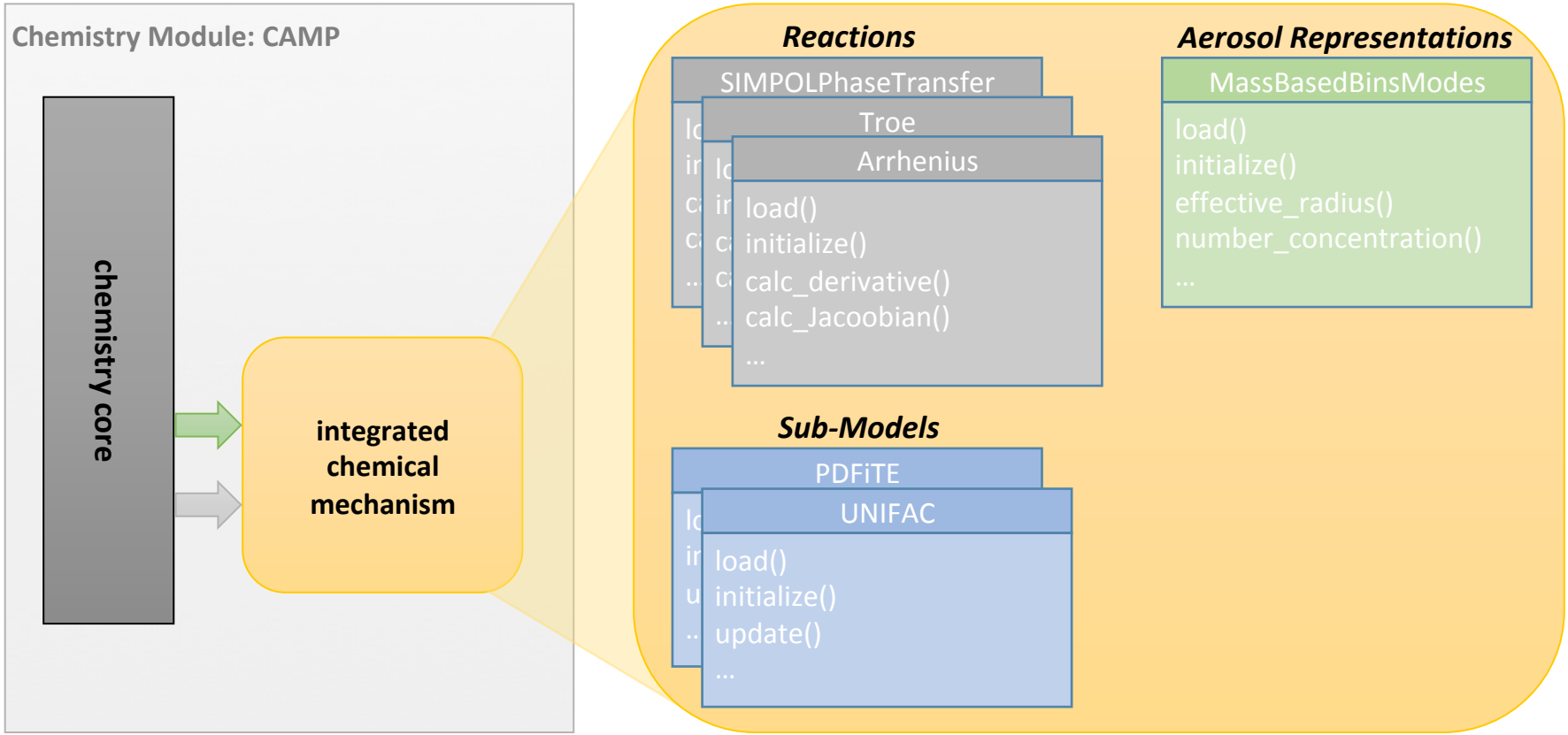


JSON Configuration Files

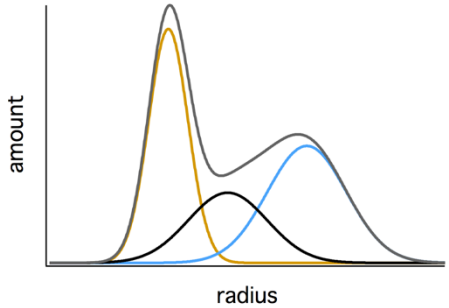
- Readily applied to science models
- Industry standard – lots of free tools available



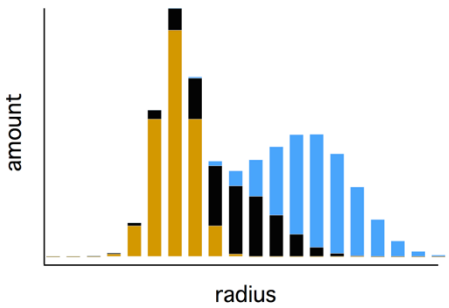
Object-Oriented Design



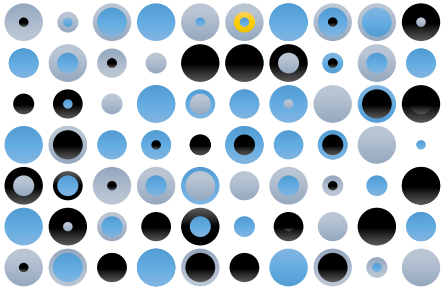
Aerosol Representations in Chemical Models – Challenges



Modal

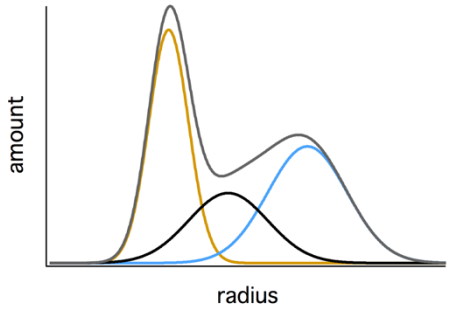


Binned



Particle Resolved

Aerosol Representation Abstraction – Approach



Modal

```
{
  "name" : "Modal",
  "type" : "AERO_REP_MODAL_BINNED_MASS",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
          ]
      }
    }
  }
}
```

INPUT

Modal
load() initialize() effective_radius() number_concentration() …

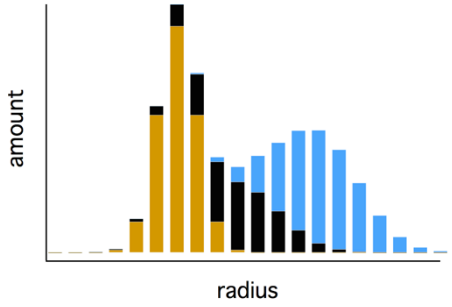
Model State

- gas-phase species
- BC — mode 1 – black carbon
- O — mode 2 – organics
- I — mode 3 – inorganics

INPUT

AerosolPhase
load() initialize() …

Aerosol Representation Abstraction – Approach



Binned

```
{
  "name" : "Binned",
  "type" : "AERO_REP_MODAL_BINNED_MASS",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
          ]
      }
    }
  }
```

INPUT

Binned
load() initialize() effective_radius() number_concentration() …

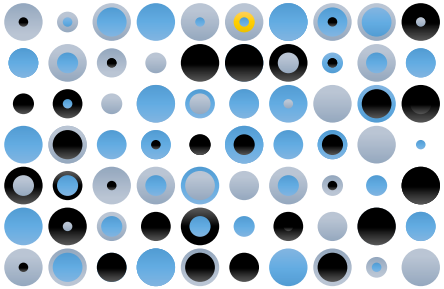
Model State

- gas-phase species
- BC — bin 1 – black carbon
- O — bin 1 – organics
- I — bin 1 – inorganics
- BC — bin 2 – black carbon
- O — bin 2 – organics
- I — bin 2 – inorganics
- bin 3 – …

INPUT

AerosolPhase
load() initialize() …

Aerosol Representation Abstraction – Approach



Particle Resolved

```
{
  "name" : "Particle Resolved",
  "type" : "AERO_REP_PARTICLE_RESOLVED",
  {
    "name" : "inorganics",
    {
      "name" : "black carbon",
      {
        "name" : "organics",
        "type" : "AERO_PHASE",
        "species" : [
          "PM_phob", "PM_phil", "ISOP-P1_aero",
          "ISOP-P2_aero", "TERP-P1_aero", "TERP-P2_aero"
          ]
      }
    }
  }
```

INPUT

ParticleResolved

load()
initialize()
effective_radius()
number_concentration()
…

Model State

- gas-phase species
- BC particle 1 – black carbon
- O particle 1 – organics
- I particle 1 – inorganics
- BC particle 2 – black carbon
- O particle 2 – organics
- I particle 2 – inorganics
- particle 3 – …

INPUT

AerosolPhase

load()
initialize()
…

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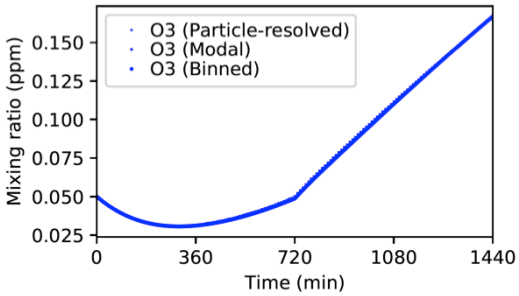
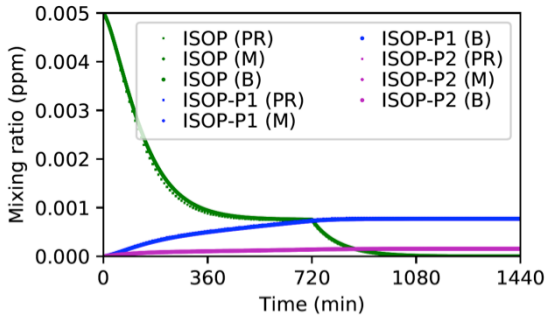
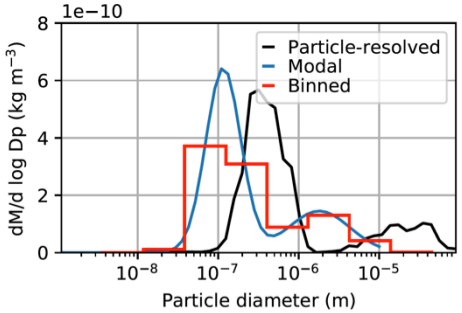
Results with different aerosol representation assumptions

- **Box model scenario**
  - CB05 gas-phase chemical mechanism + two-product Isoprene SOA formation
  - 24h integration, photolysis on and emissions on first 12h
  - Three cases with different aerosol representation: modal, binned, particle resolved
    - Fixed size distribution parameters modal and binned cases

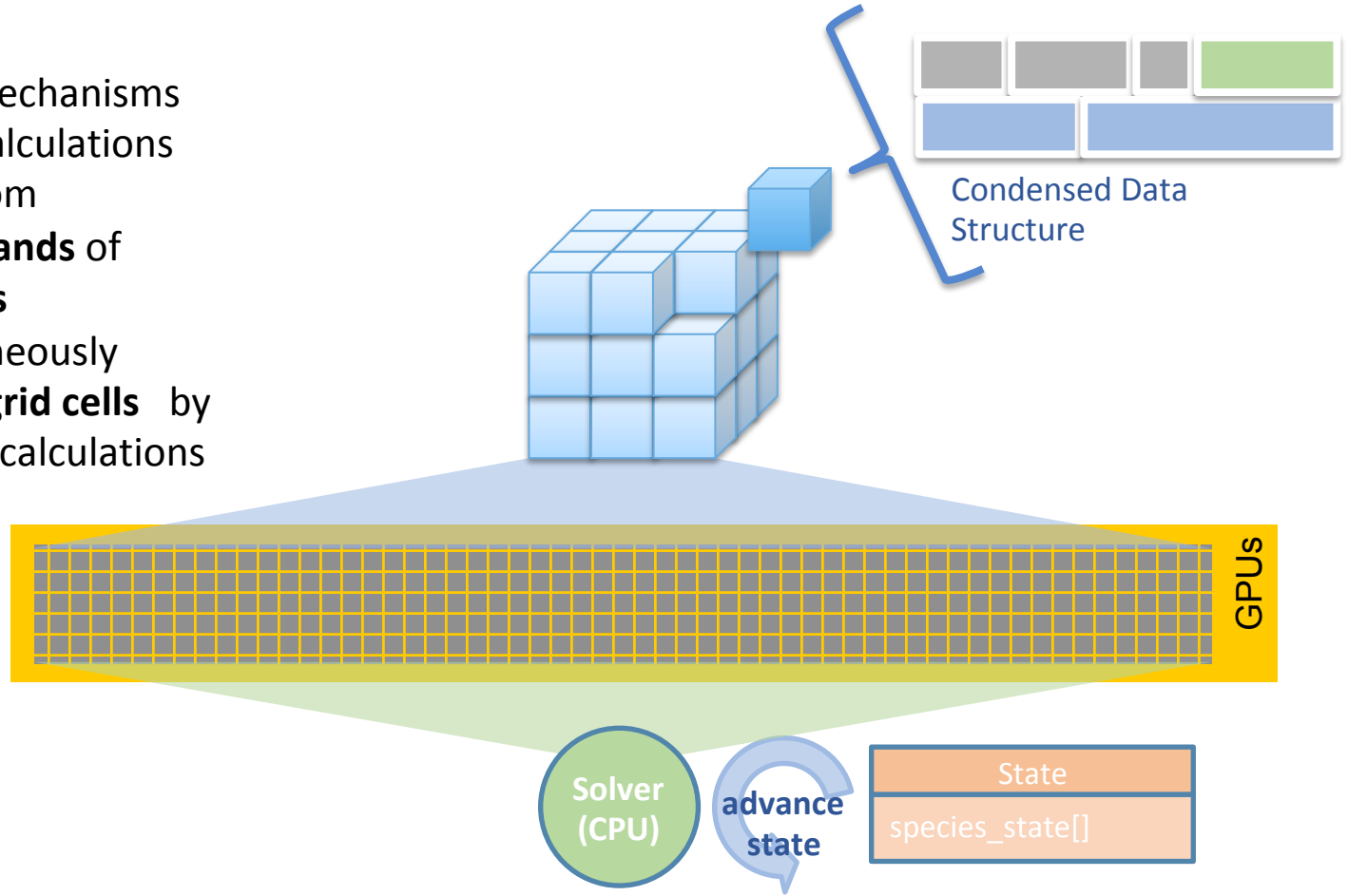






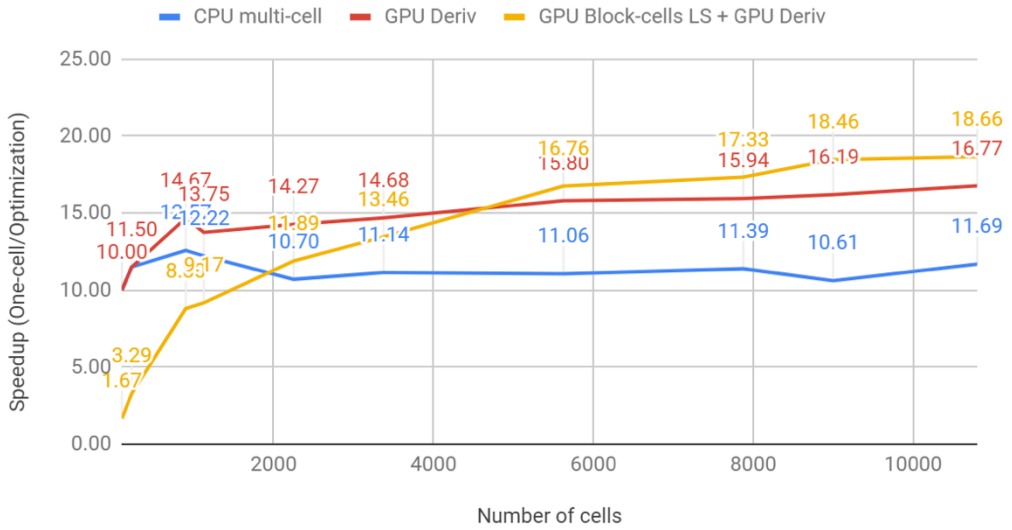
Porting to GPUs

- Solving chemical mechanisms involve repeated calculations of contributions from **hundreds** or **thousands** of individual **reactions**
- Approach: simultaneously solve for **multiple grid cells** by spreading reaction calculations across GPUs



GPU results

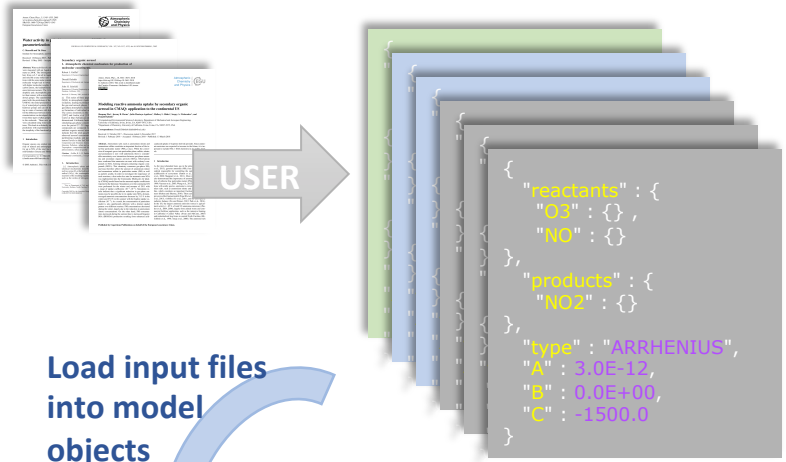
- Near 30% of the computational load on CPU has been translated to GPU:
  - F(y) function
  - Linear solving process



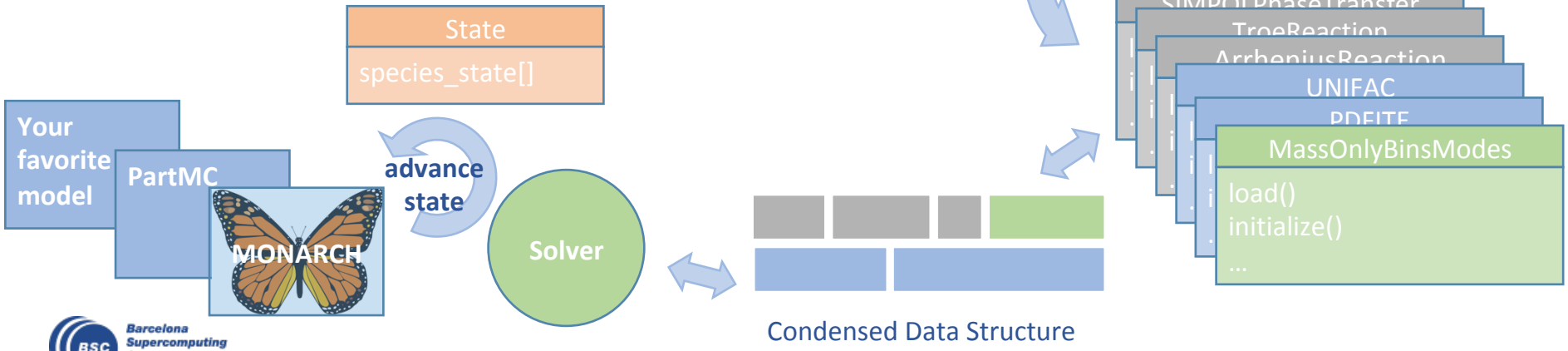
Configuration: simple mechanism with similar initial concentrations among cells

Chemistry Module – Overall Workflow

- Change the chemical mechanism ***without recompiling***
  - Vary mechanism complexity based on conditions/location
  - Compare mechanisms in real time
- Use ***same mechanisms*** across models (MONARCH, PartMC, etc.) changing only **Aerosol Representation** JSON



Load input files into model objects



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The PartMC library is available at: `https://github.com/compdyn/partmc`

NCAR UCAR National Center for Atmospheric Research

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ILLINOIS

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AXA Chair on Sand and Dust Storms

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