Workflow Optimization & Processing of Complex Datasets for Off-site Fusion Energy Research

A. Wingen, E.A. Unterberg, J.H. Harris, J.C. Hill, S.P. Hirshman, S.K. Seal

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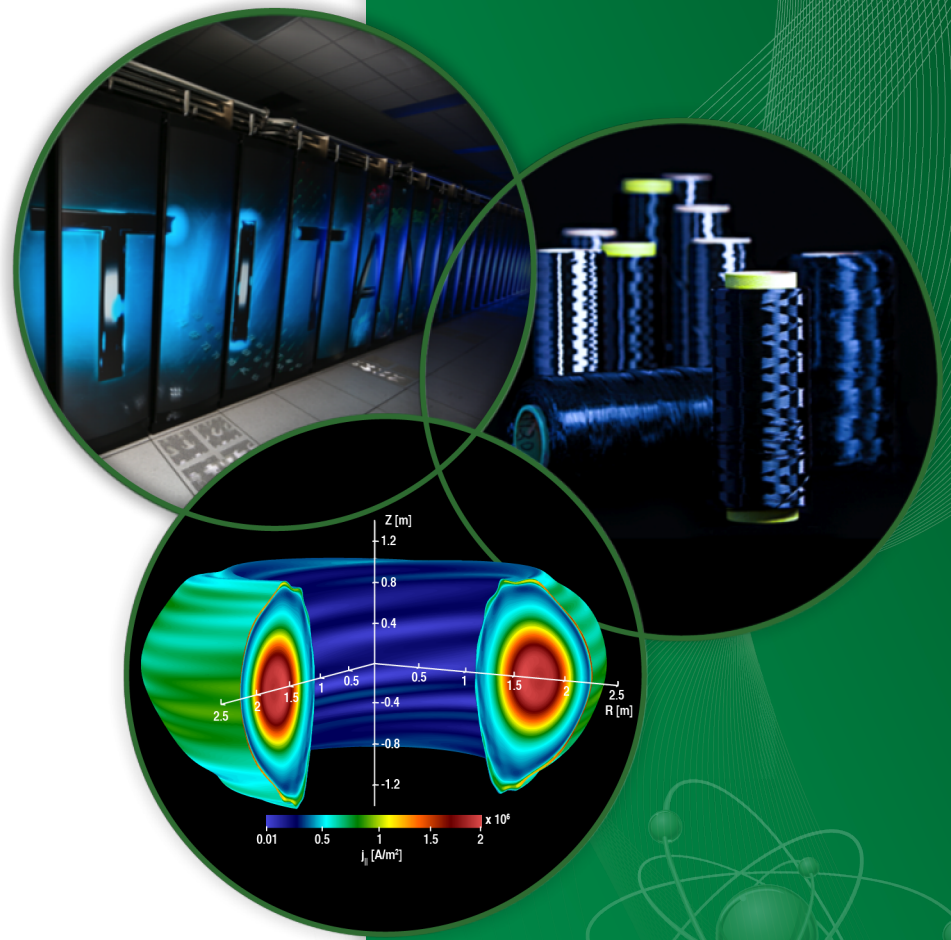

presented at:
ORNL, November 11. 2014

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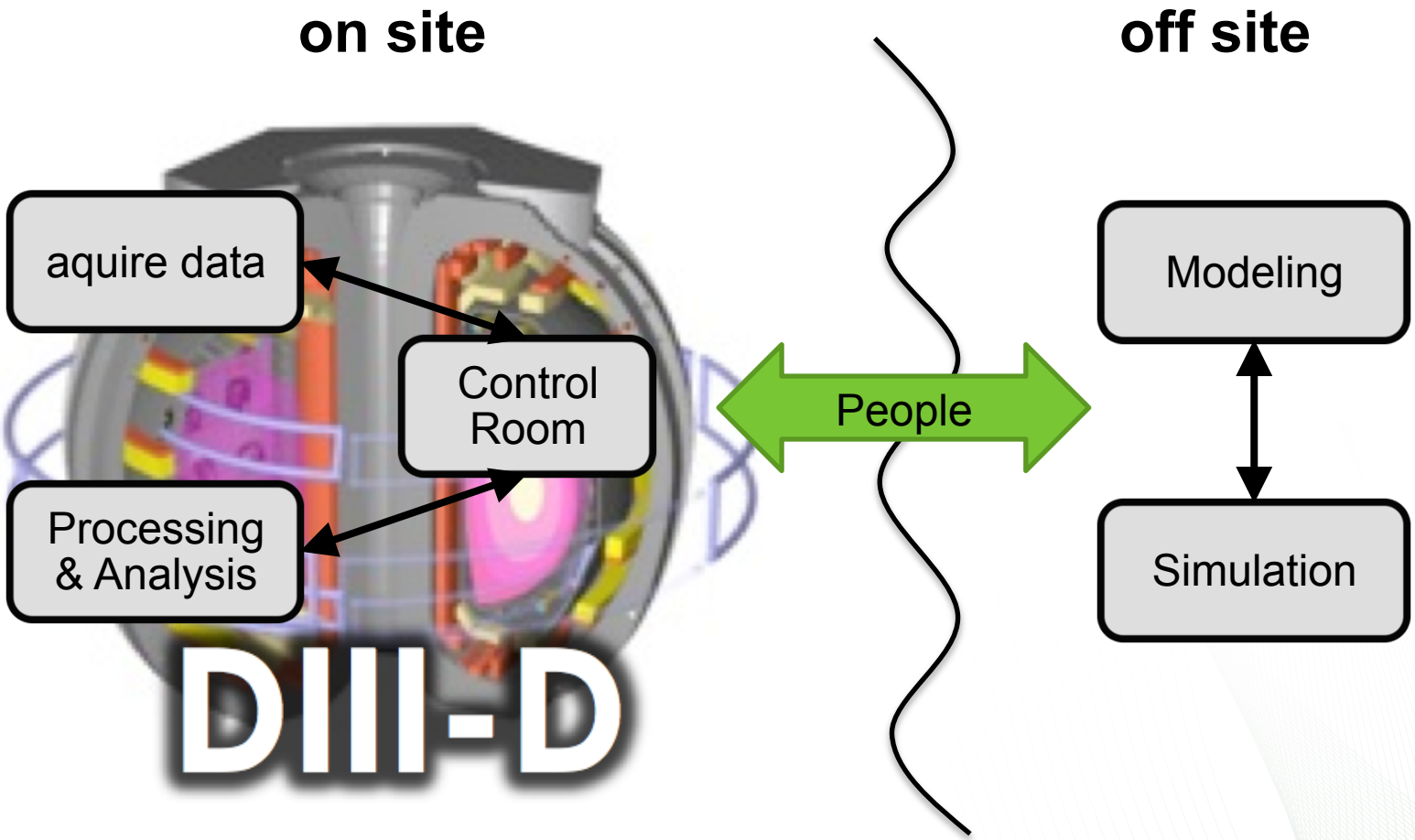
Collaborative experimental workflows in fusion today focus on control room interaction



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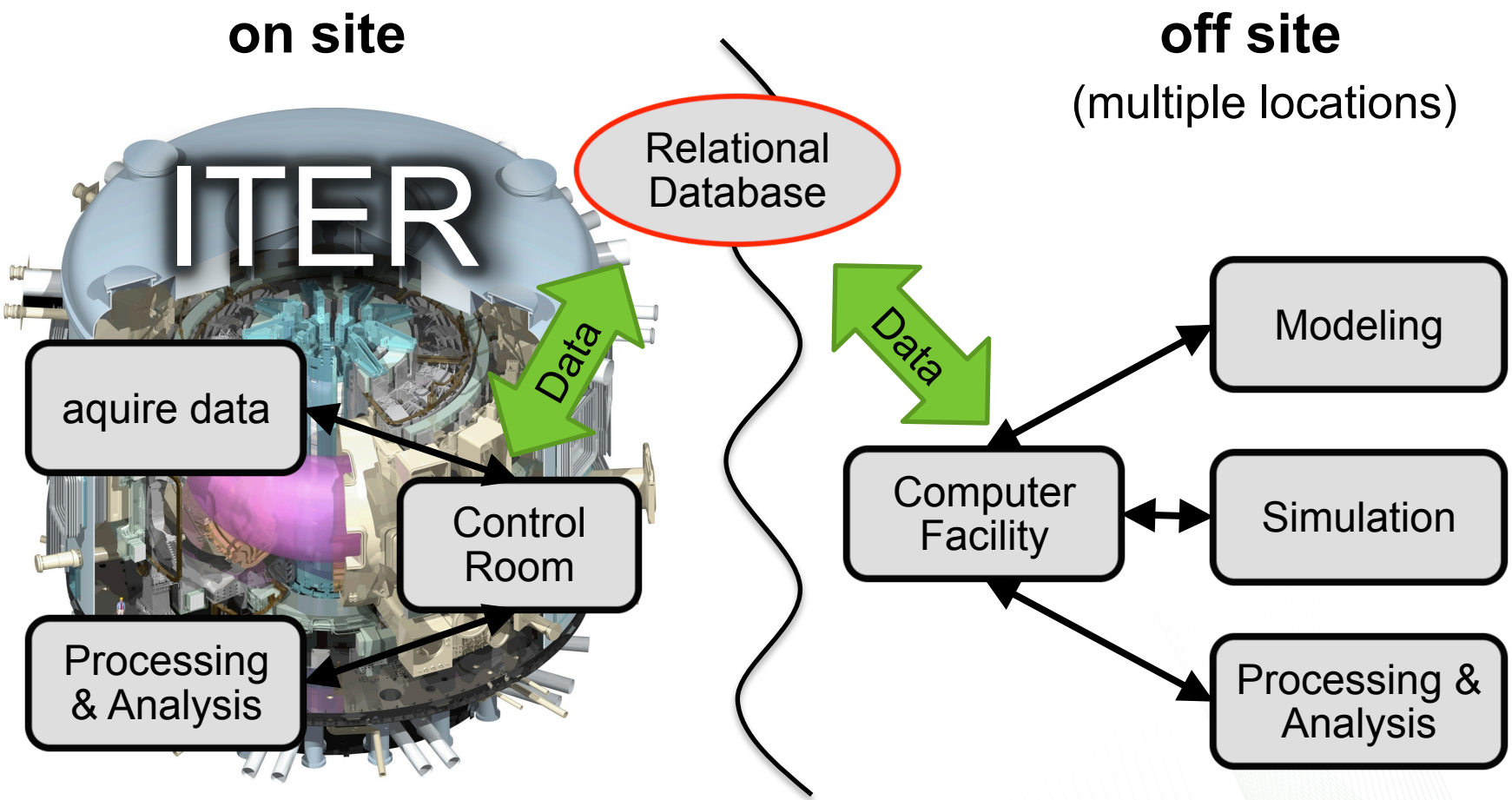
In ITER era collaborative tools will be essential



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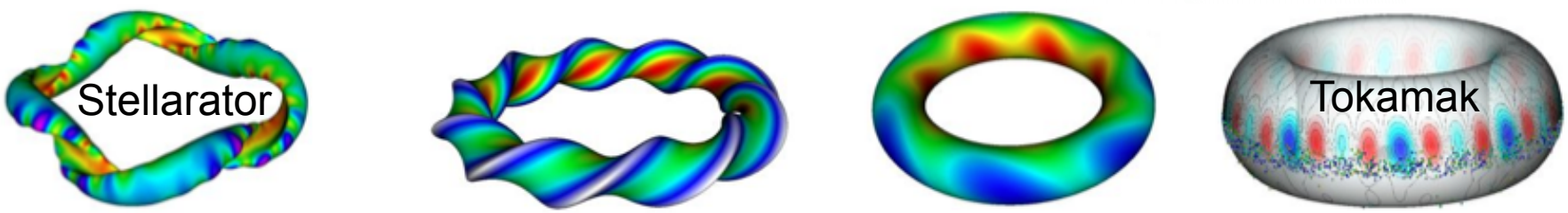
Develop off-site data analysis/transfer capability to inform a run-day

- **Implement a toolset to optimally reconstruct 3-D equilibria of H-mode tokamak discharges**
- **Couple toolset to a single DIII-D run-day**
  - *take data*
  - *analyse off-site*
  - *transfer to off-site*
  - *give feed back to experiment*
- **Project aims to leverage ORNL core strengths to position US for a leadership role in ITER analysis**
  - *long history in developing 3-D tools for stellarators*



strongly 3-D
well developed

3-D codes

weakly 3-D
still developing

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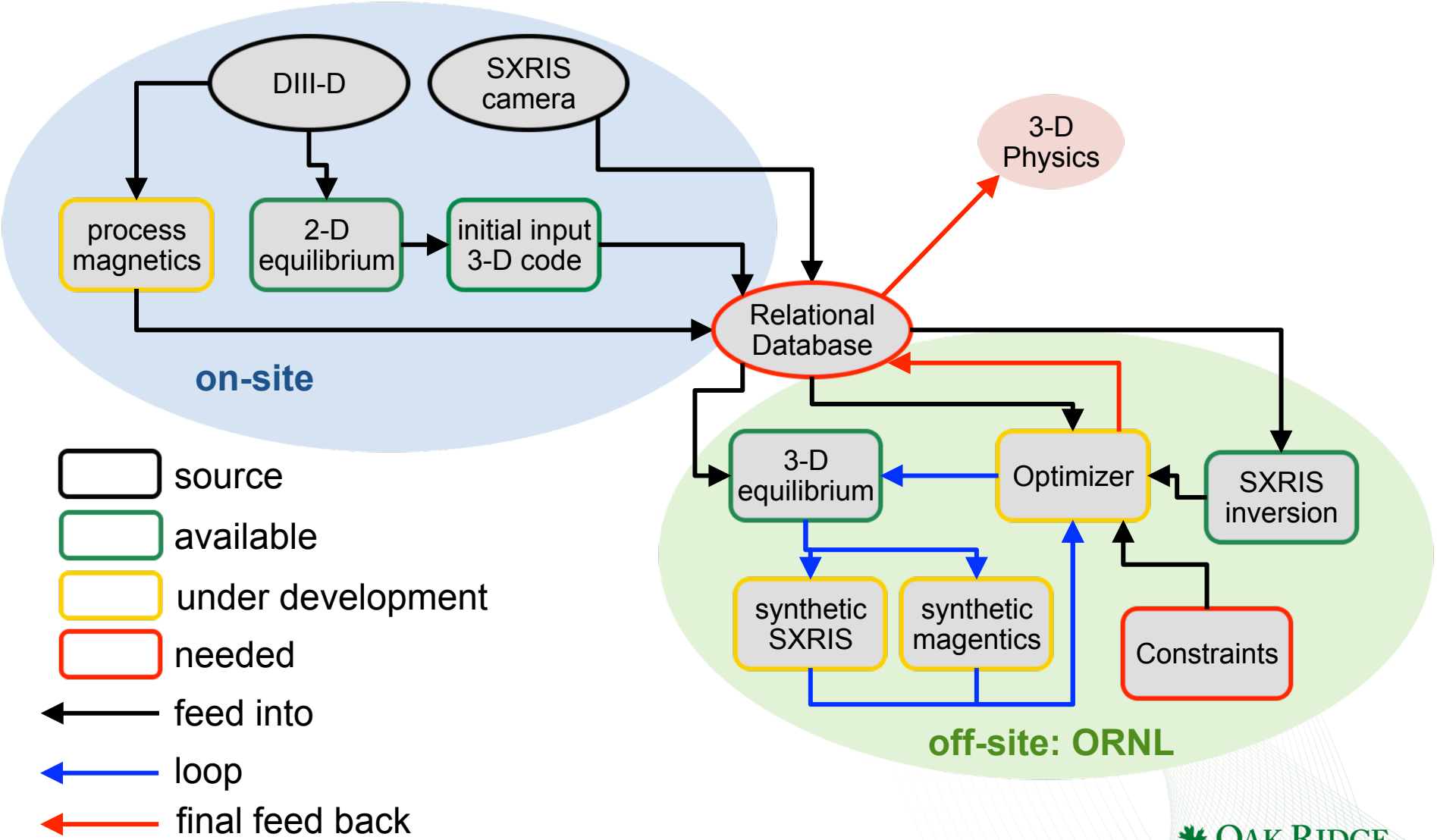
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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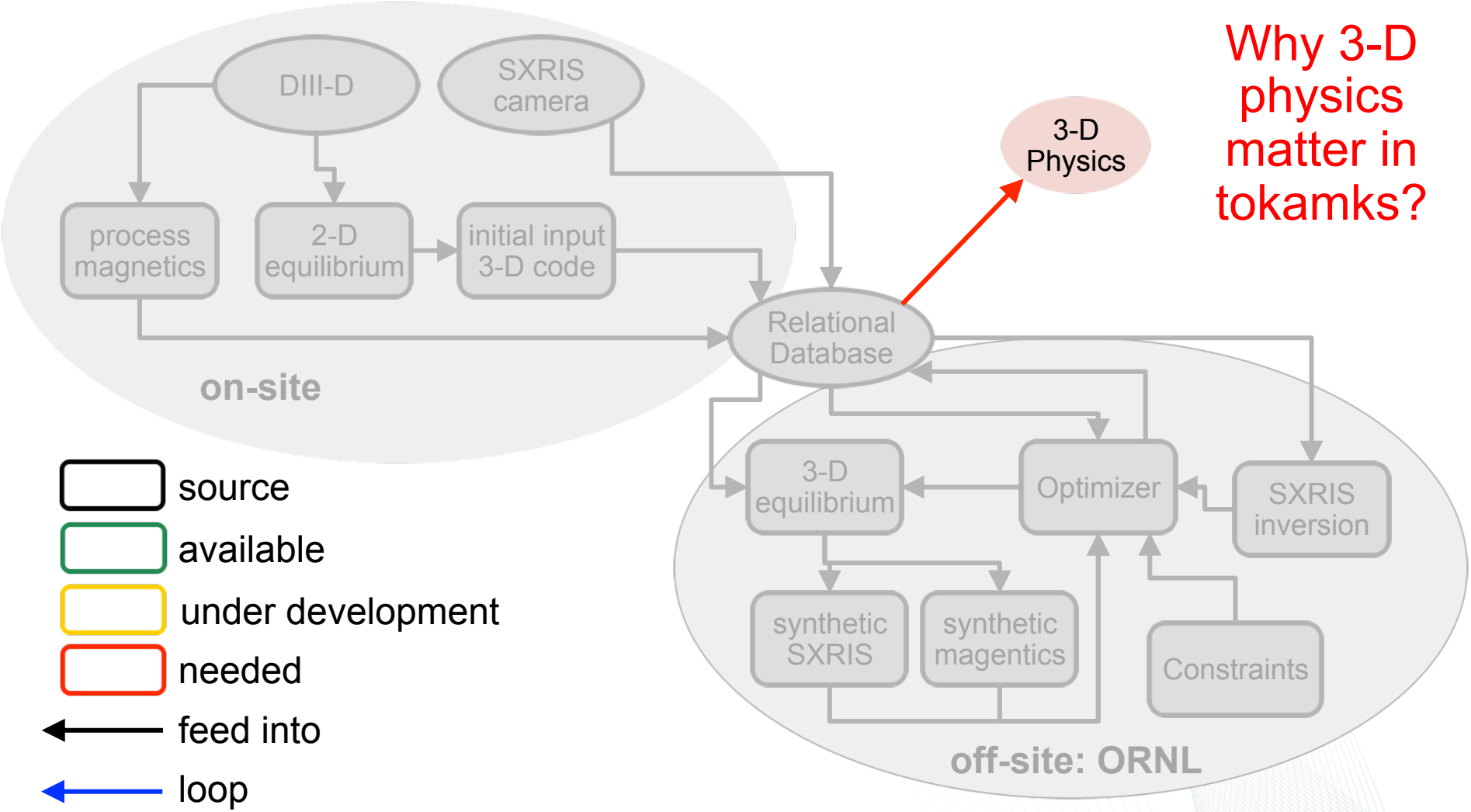

Why 3-D physics matter in tokamks?

- source
- available
- under development
- needed
- feed into
- loop
- final feed back

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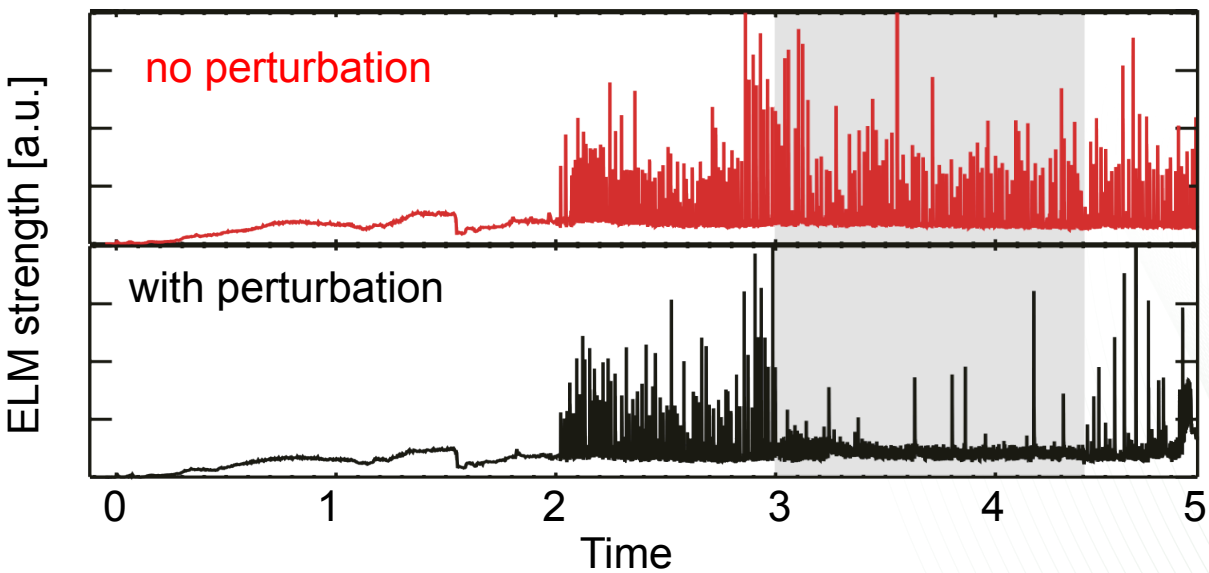
Small (~10^{-3}), external, 3-D, magnetic-field perturbations can stabilize tokamak edge

- **Naturally, rapidly occuring edge instabilities, ELMs, can melt or erode plasma facing components in ITER**

A. Loarte *et al.*, PPCF **45** , 1549 (2003)

- **3-D perturbations successfully control ELMs in DIII-D and other tokamaks**

T.E. Evans *et al.*, PRL **92** , 235003 (2004)



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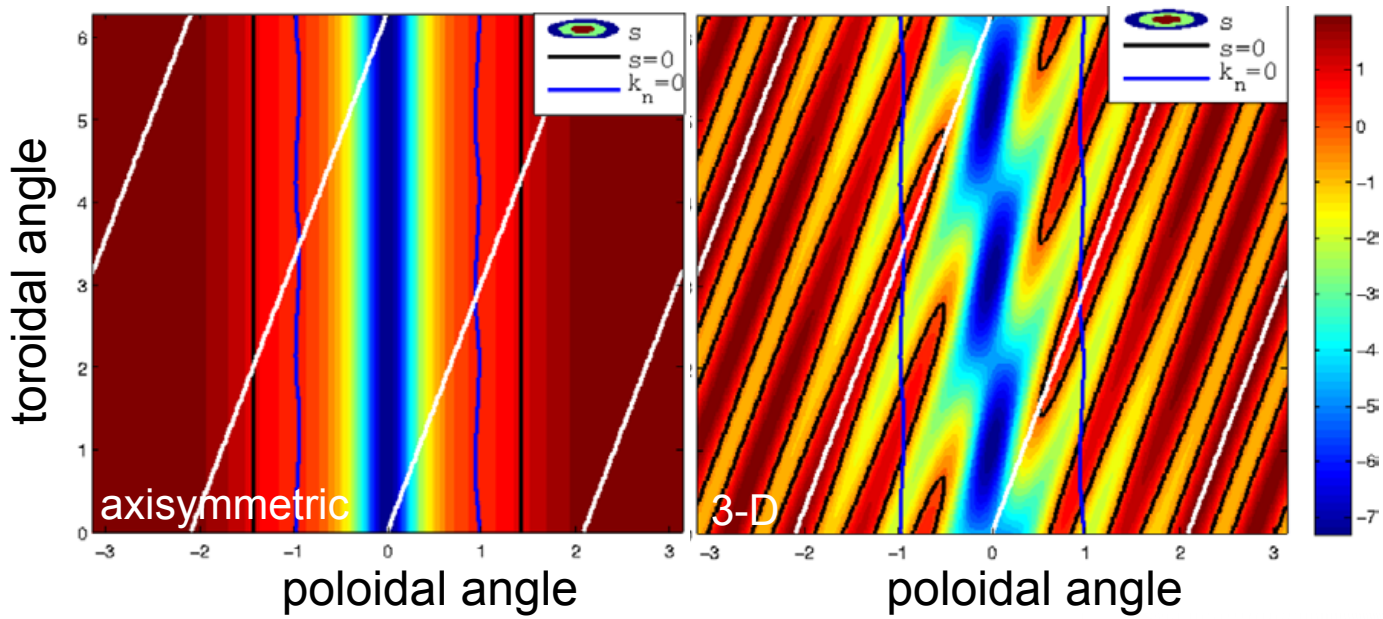
3-D fields have a significant effect on geometric coefficients, like local shear

T.M. Bird *et al.*, NF **53**, 013004 (2013)



- **Hypothesis: Zero shear at negative curvature drives ideal ballooning micro-turbulance**
  → enhanced transport limits pedestal growth
  → ELMs are stabilized

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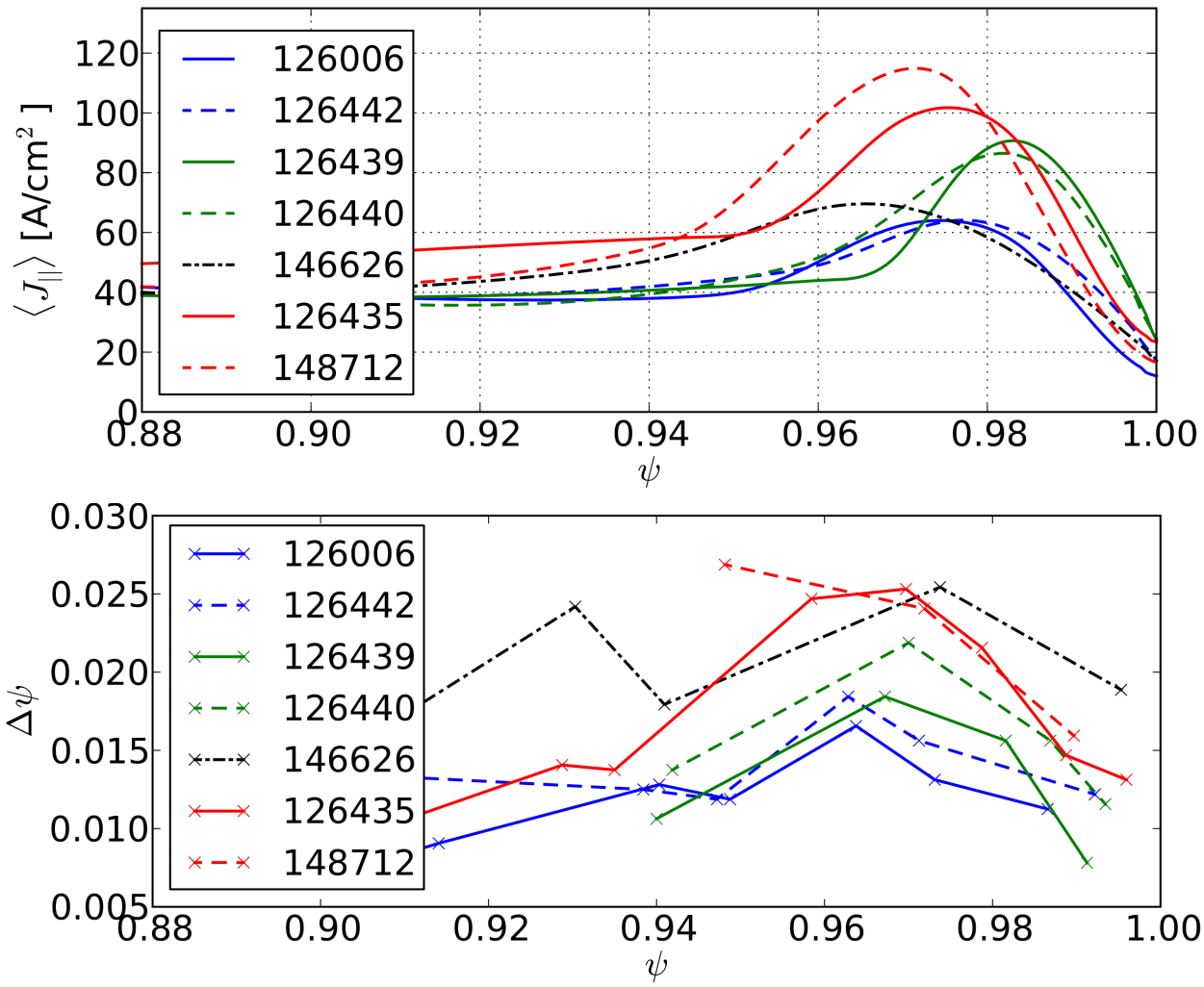
Linear resistive MHD shows: Kink displacements follow current density

- **low edge current**
  - *small displacements*
  - *island like*
- **moderate current**
  - *intermediate*
- **strong current**
  - *large displacements*
  - *kink like*
  - ***ELMs return***



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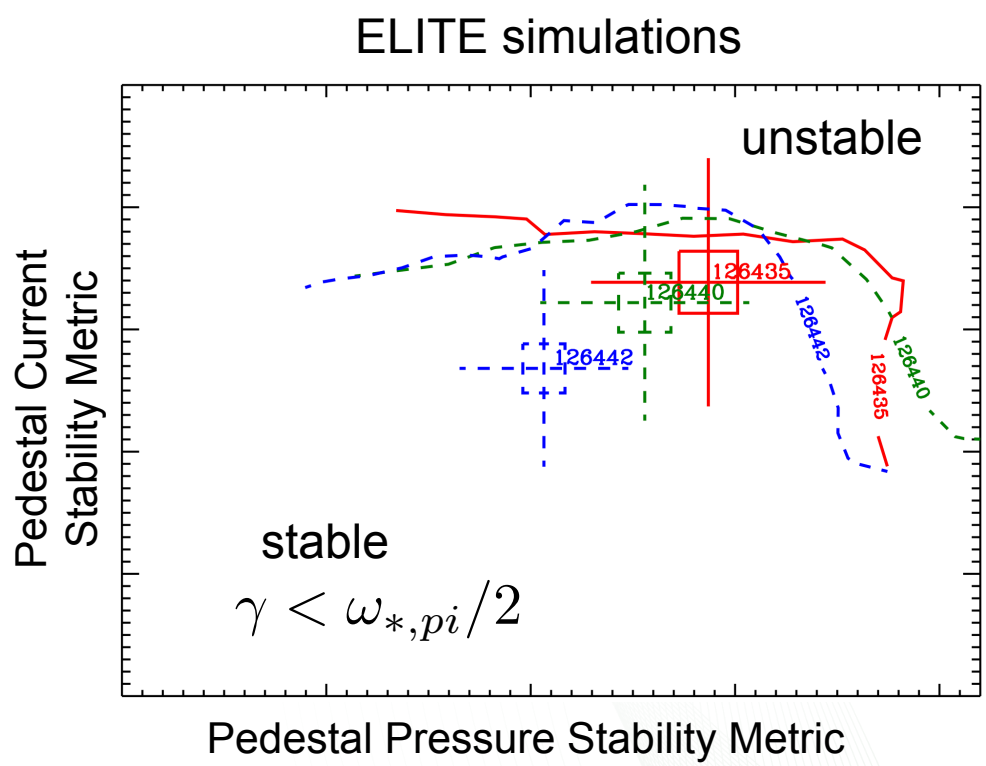
Hypothesis: Discharges with stronger Kink response are closer to peeling ballooning stability threshold

- **well suppressed**
- **good suppression but at higher perturbation**
- **Marginally stable**
  - *only mitigation*
  - *ELMs intermittendly return*
- **Order follows kink displacements**



A. Wingen *et al.*, EPS **P5.029** (2014)

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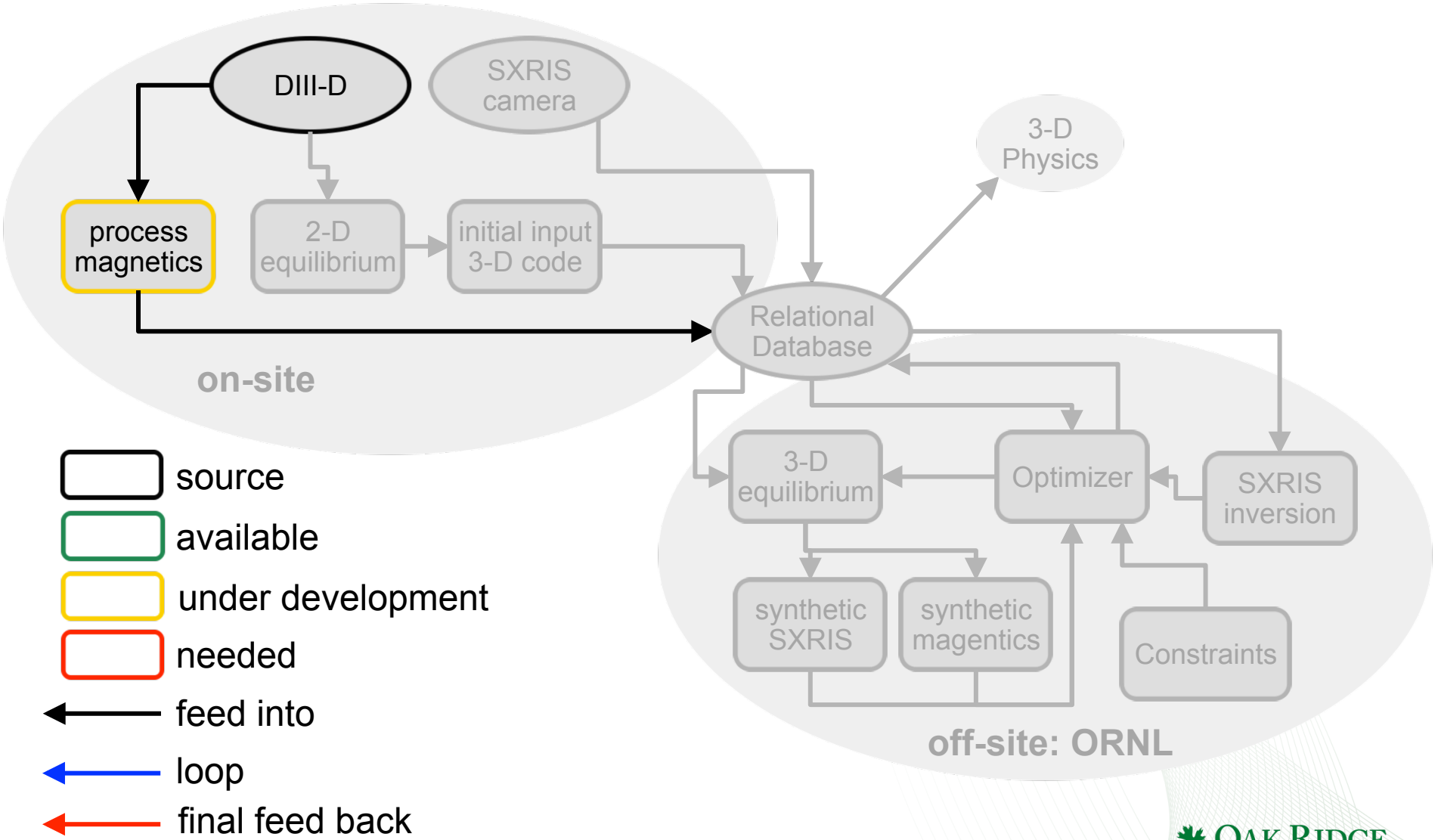
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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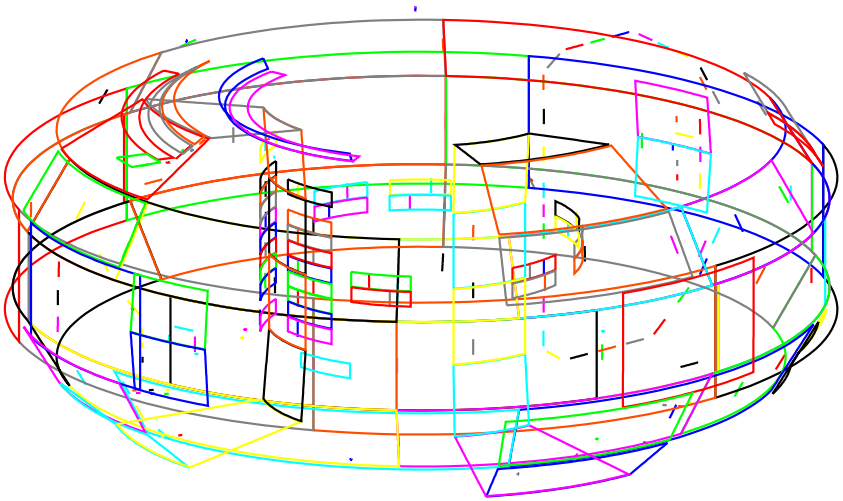
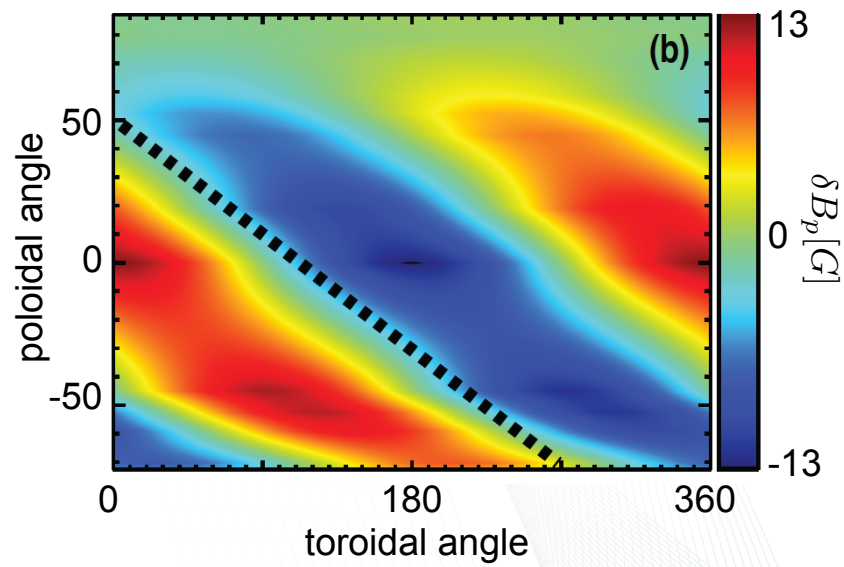
Exploit DIII-D's good 3-D diagnostic capability

- **250 magnetic probes + 120 differenced pairs measure 3-D plasma response at the wall**
  - *here:* δB_p *of a rotating m/n = 2/1 tearing mode at LFS*



J.D. King *et al.*, RSI **85, 083503 (2014)**



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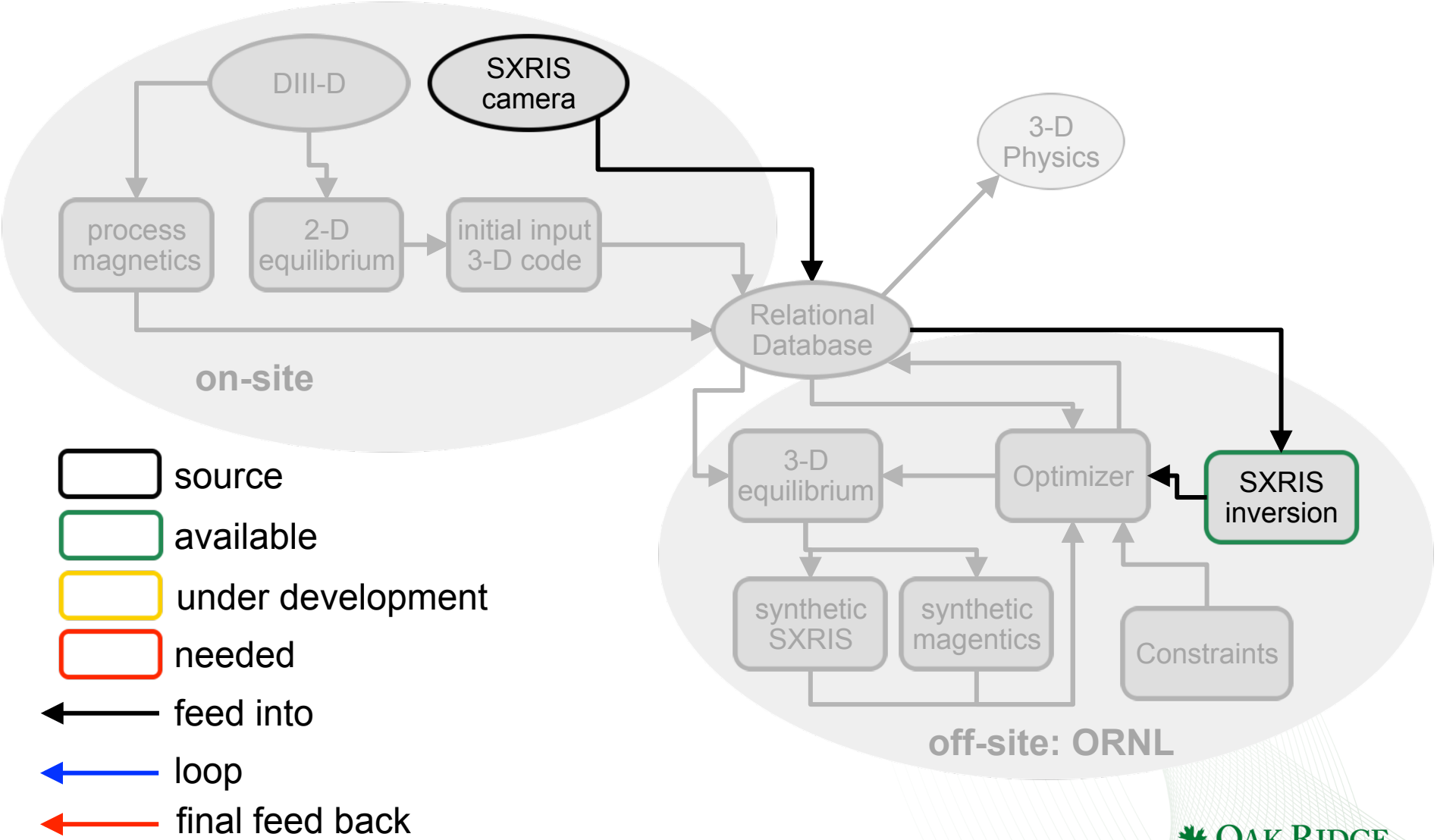
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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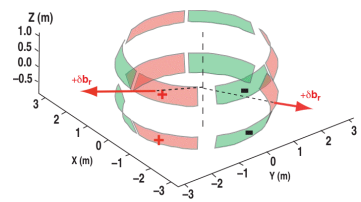
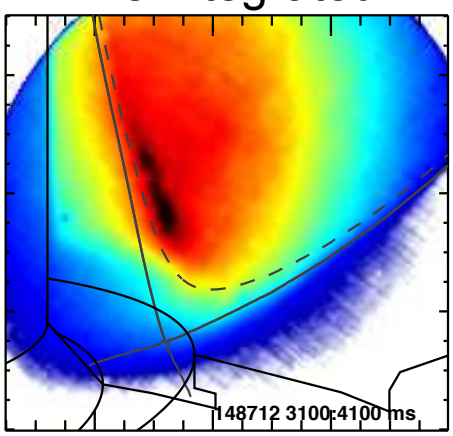
Tangential soft X-ray imaging reveals 3-D structures in the H-mode pedestal

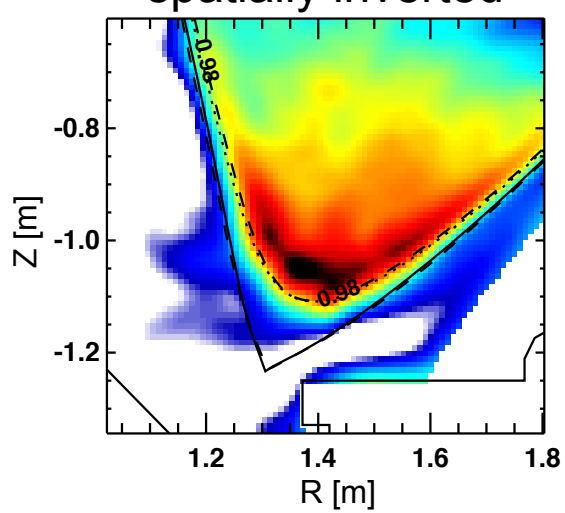
- **Soft X-Ray Imaging System (SXRIS)**
  - *line-of-sight & time integrated soft X-ray emission*
  - *spatially inverted by Tikhonov regularization* A. Wingen *et al.*, JCP, **submitted**
  - *phase differenced: n = 3 perturbation periodically flipped*



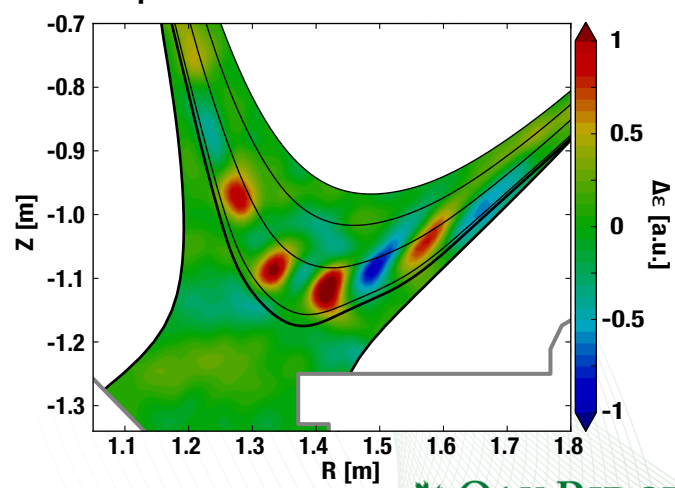
line-integrated



spatially inverted



phase differenced



A. Wingen *et al.*, NF **54**, 064007 (2014)

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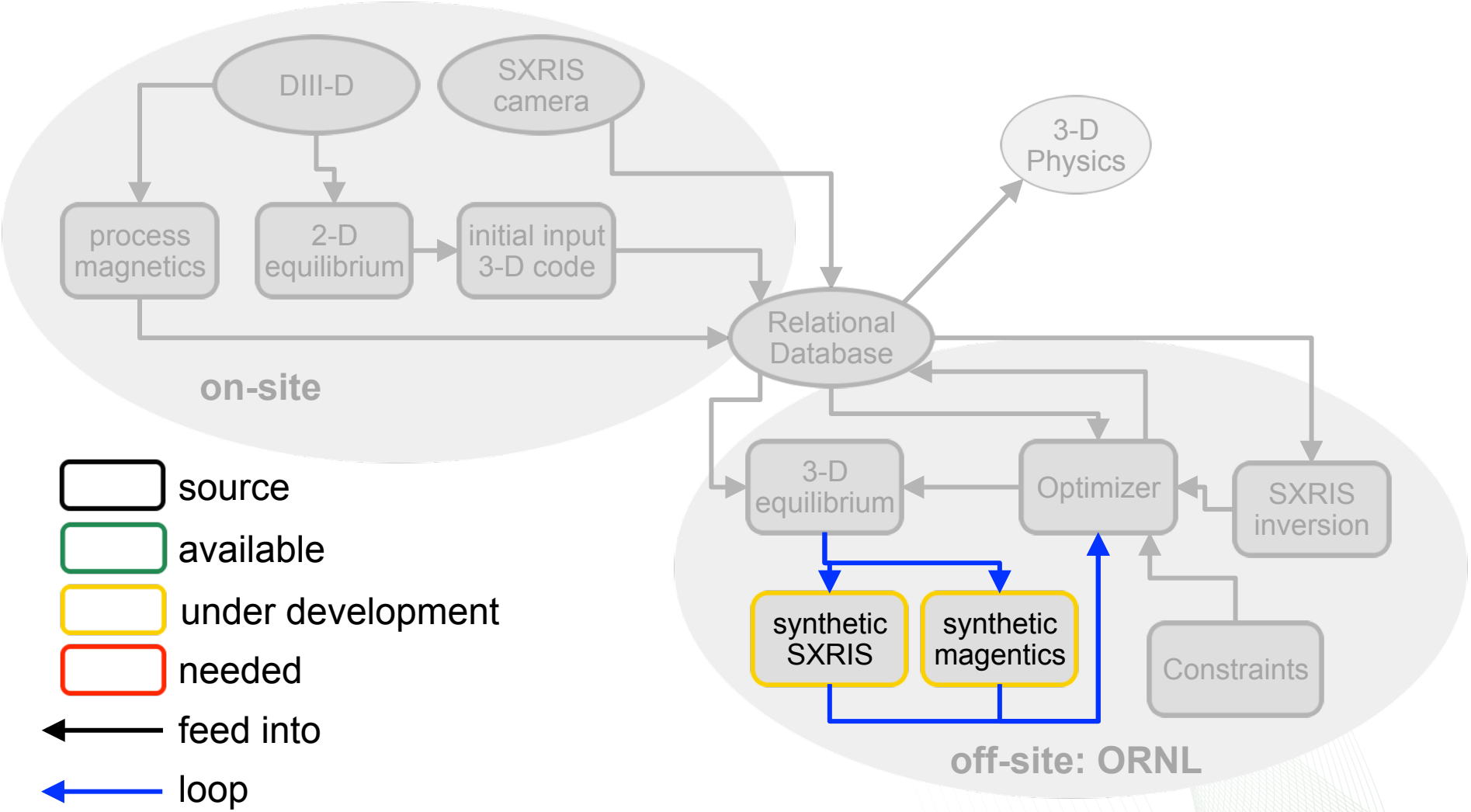
Workflow for 3-D reconstructions of H-mode DIII-D discharges



source
available
under development
needed
feed into
loop
final feed back

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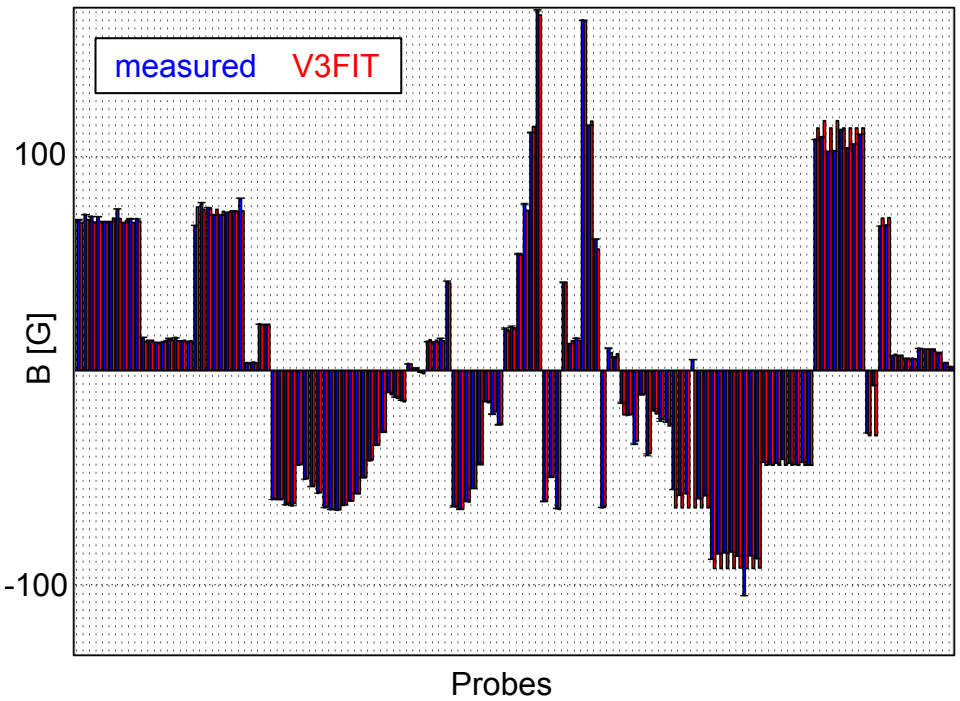
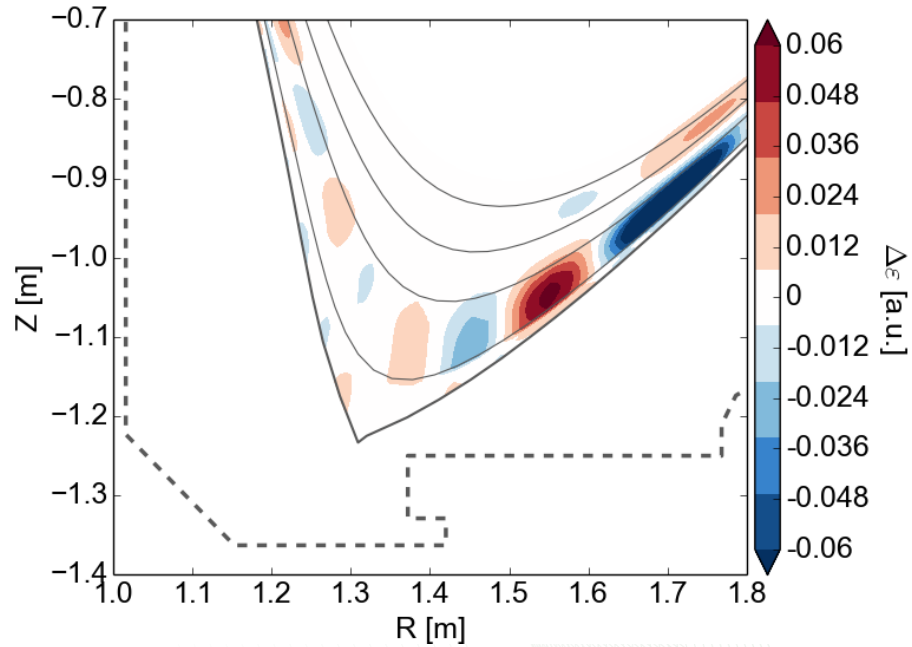
Synthetic diagnostics are under development

- **Magnetics:**
  - *Test: pulse a single poloidal field coil in vacuum*



- **SXRIS:**
  - *assining ε(ψ) to flux surfaces & subtract 0˚ and 60˚*



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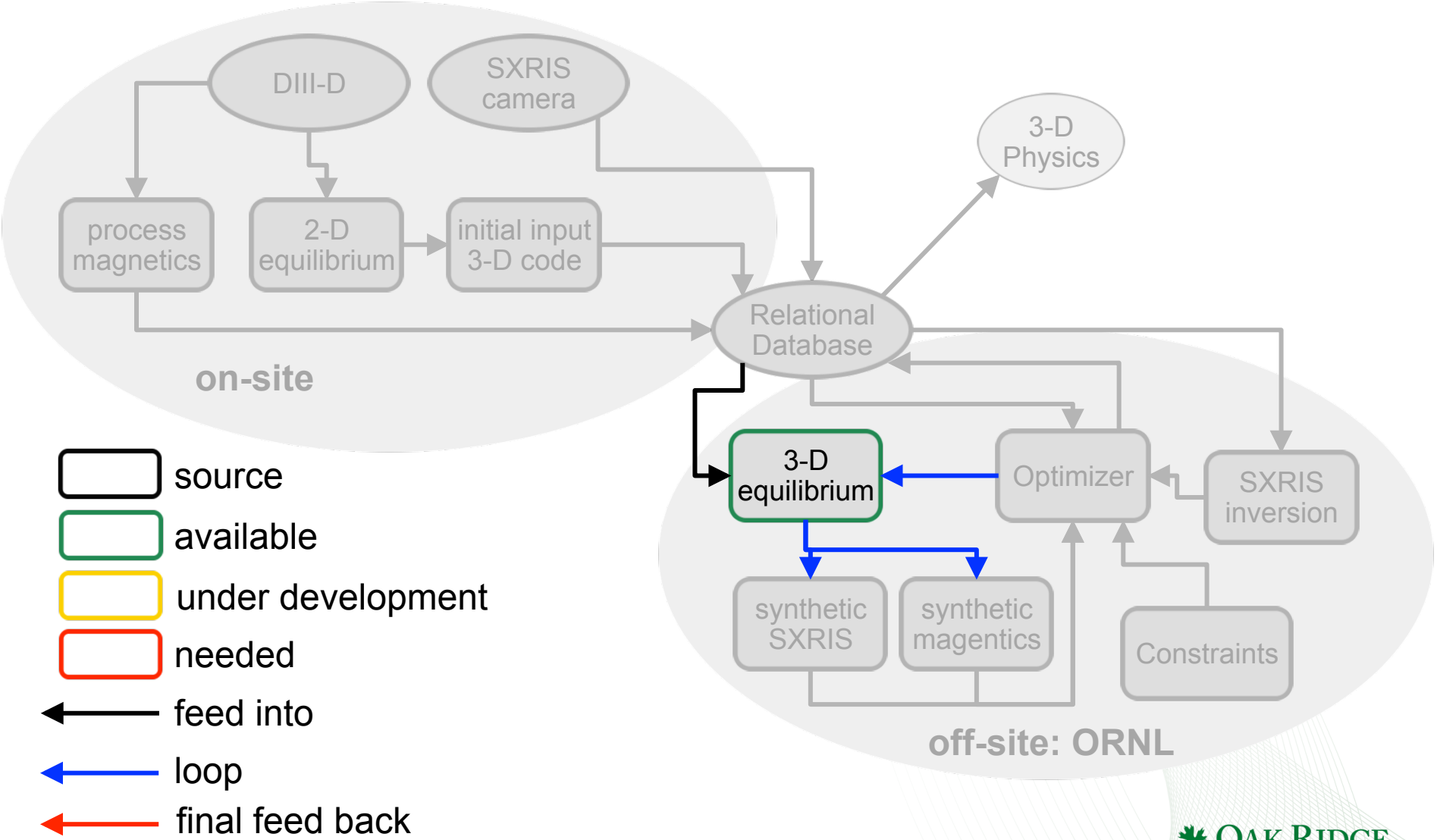
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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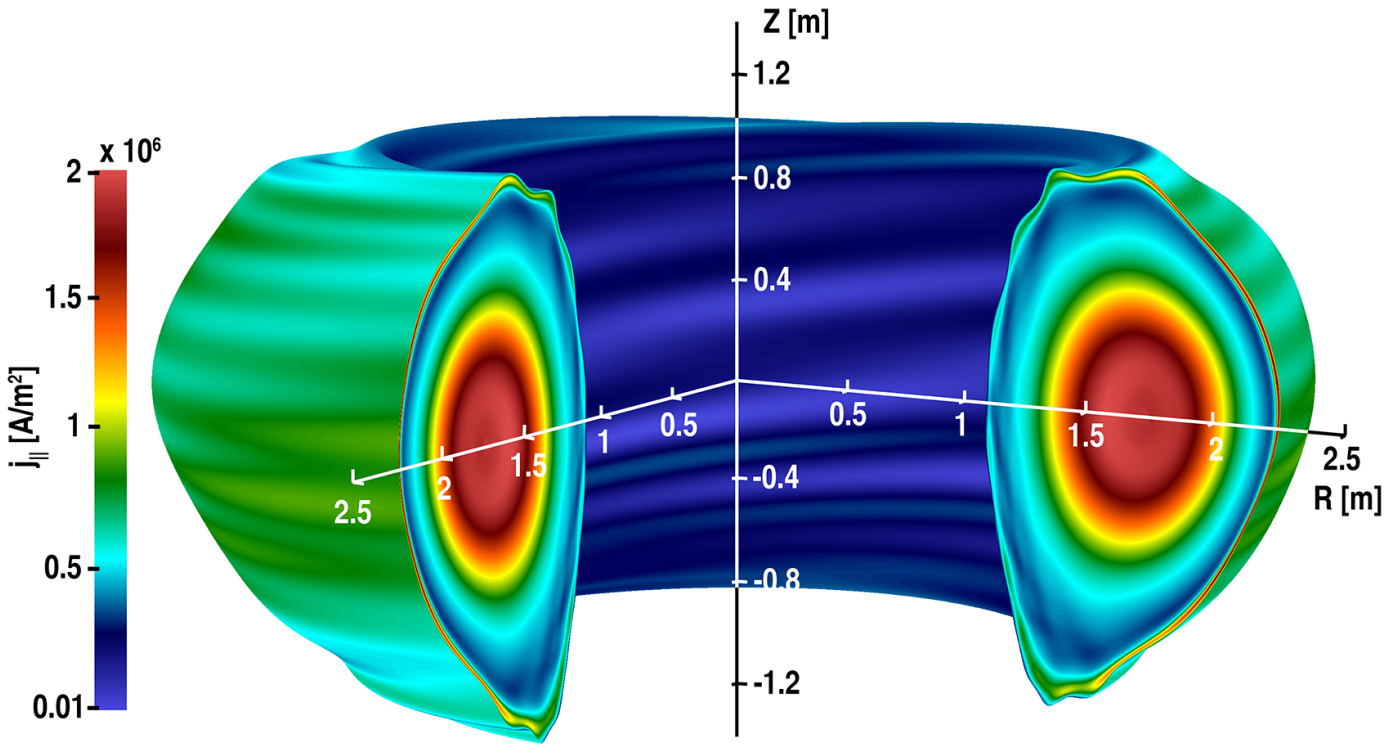
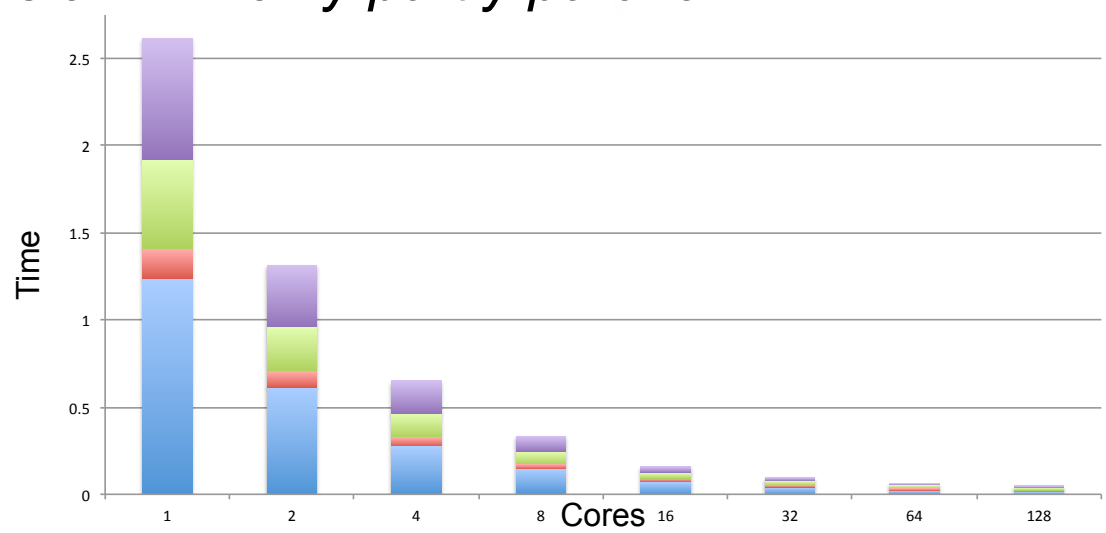
H-mode tokamak 3-D equilibria using the VMEC code

- **Ideal, non-linear MHD code → force balance**
- **Application to perturbed tokamak**
  - *weakly 3-D*
  - *up-down asymmetric*
  - *rotation*
  - *strong edge gradients*
  - *large currents*



utilize ORNL's computational hardware & expertise

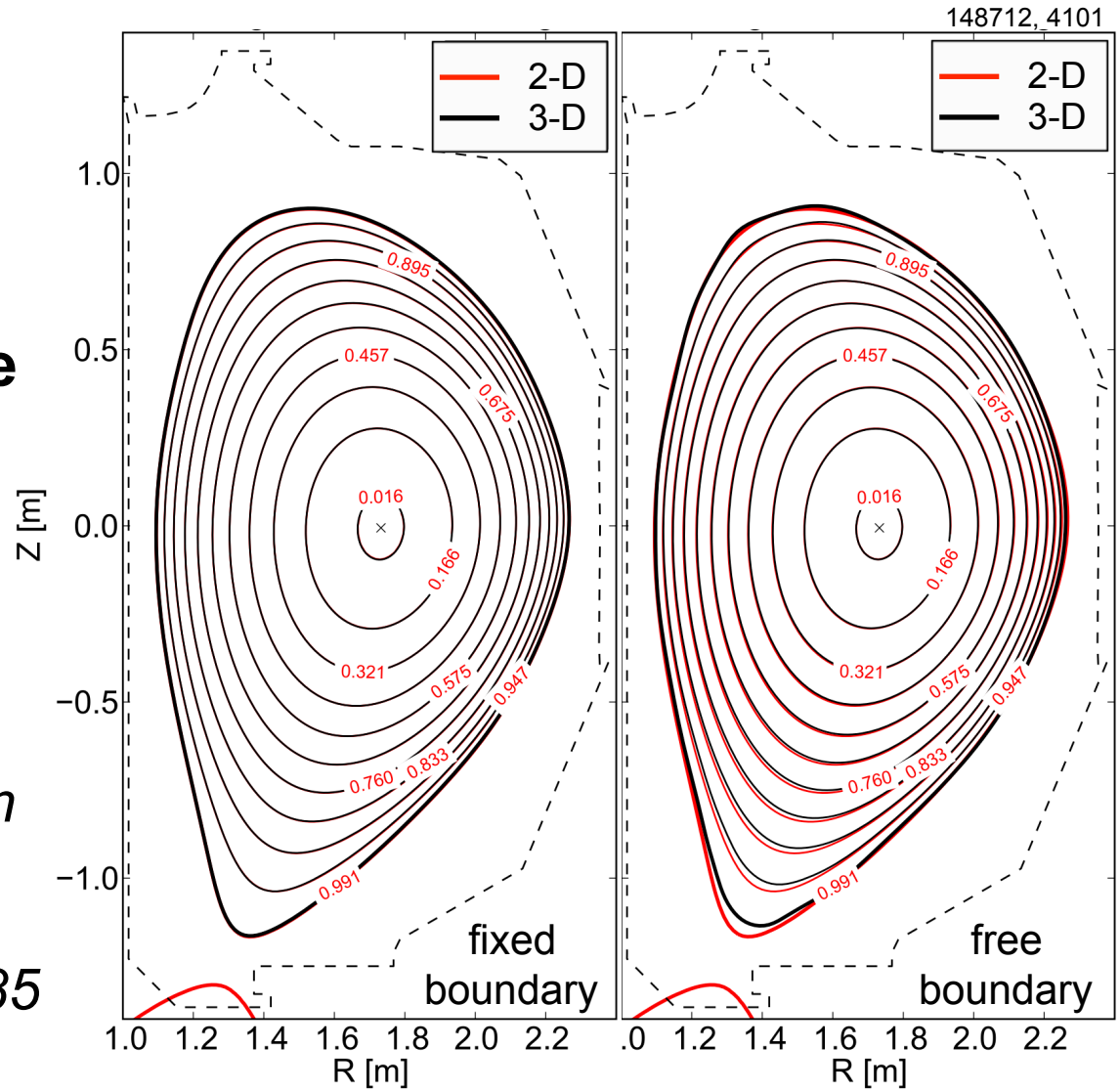
- **Resolving current sheets requires high fidelity**
  - *number of surfaces: 97, 193, 385, 769, …*
- **Effective feed-back requires fast computation**
  - *goal: within 1-3 days*
- **Both together require massive parallel runs**
  - *available: serial verison → one run takes 2 weeks*
  - *available: openMP version → only partly parallel*
  - *under construction: MPI version → fully parallel, scales on leadership class computer*



VMEC finds 3-D equilibrium

- **Use kinetic EFIT as initial condition**
  - *VMEC cannot reach separatrix → truncate*
- **Fixed boundary mode**
  - *force current profile*
  - *extract iota profile*
- **Free boundary mode**
  - *force iota profile*
  - *use iota from fixed run*
- **Here: n = 3, 3kA I-coil**
  - *n = 4, m = 32, ns = 385*

CPU time ~ 10 days



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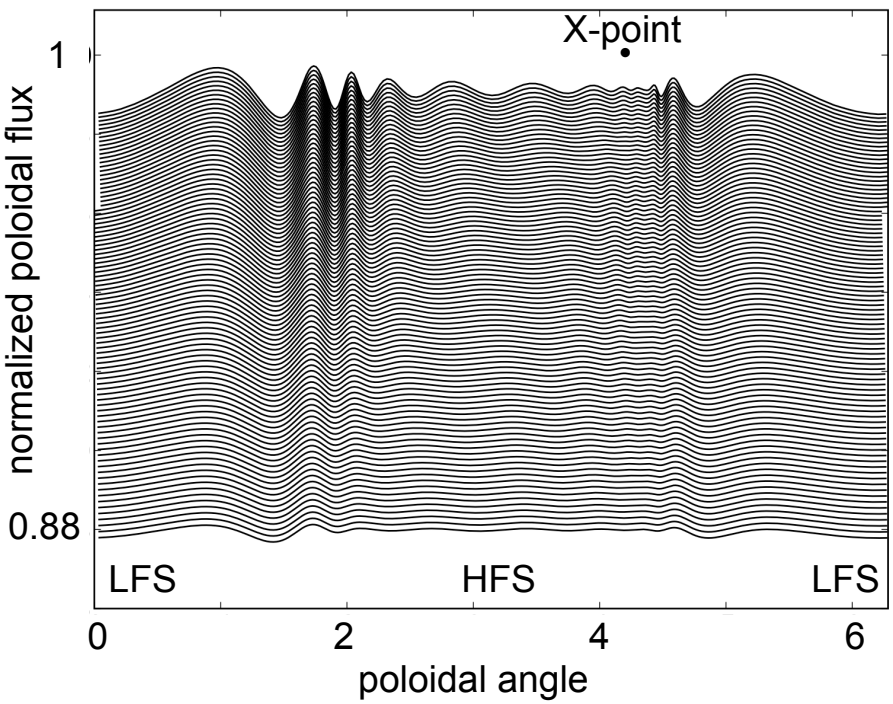
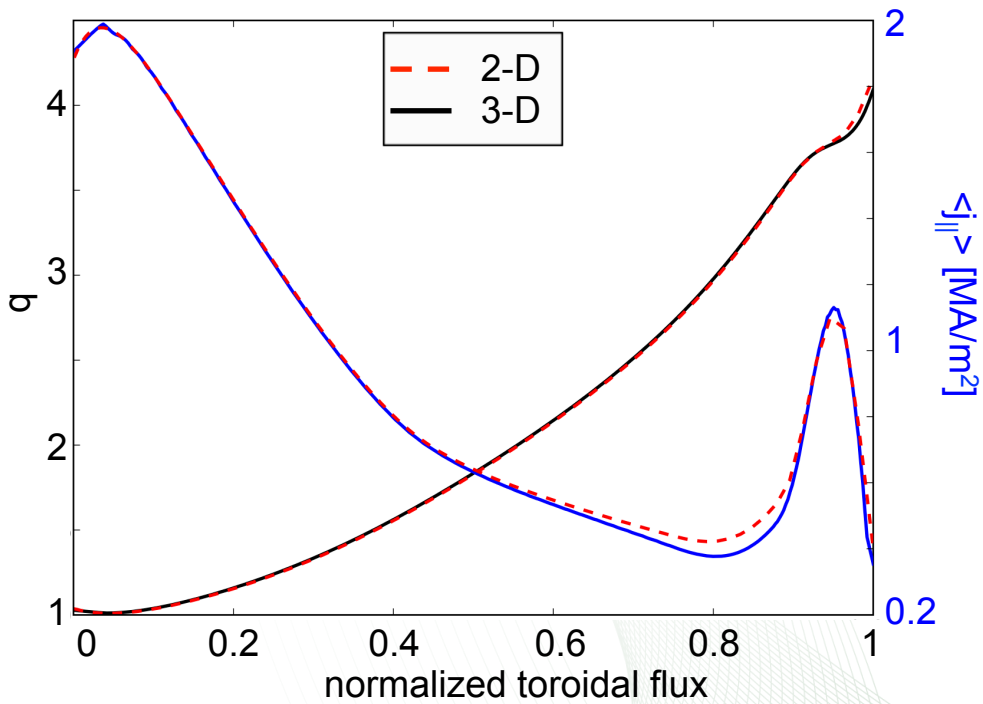
VMEC 3-D equilibrium shows characteristic n = 3 kink response to I-coil field

- **Bended flux surfaces, stabe to resolution changes**
  - *radially aligned, corrugation follows local poloidal mode number, bifurcation at X-point*
- **Flux-surface-averaged profiles close to kinetic EFIT**





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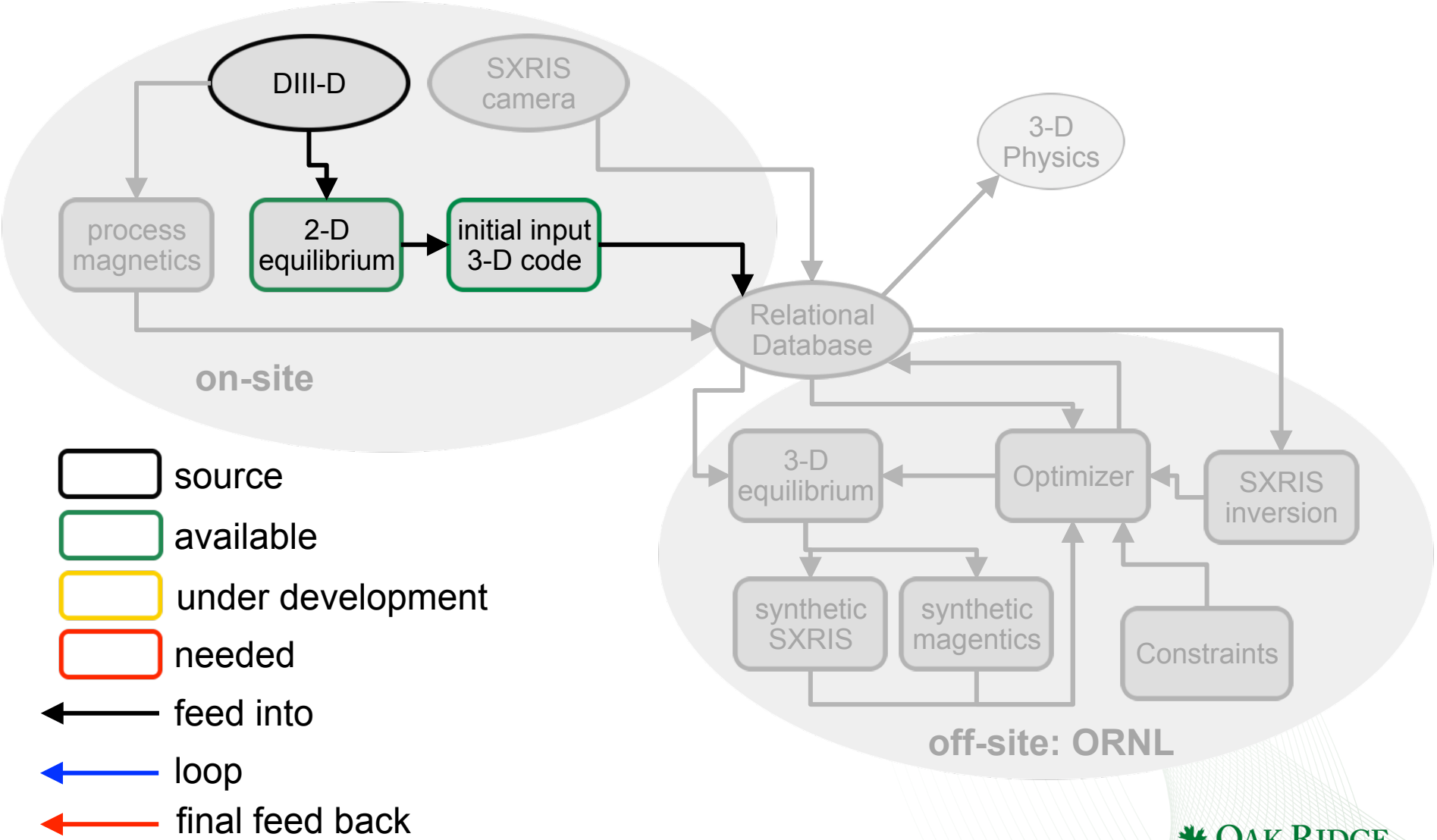
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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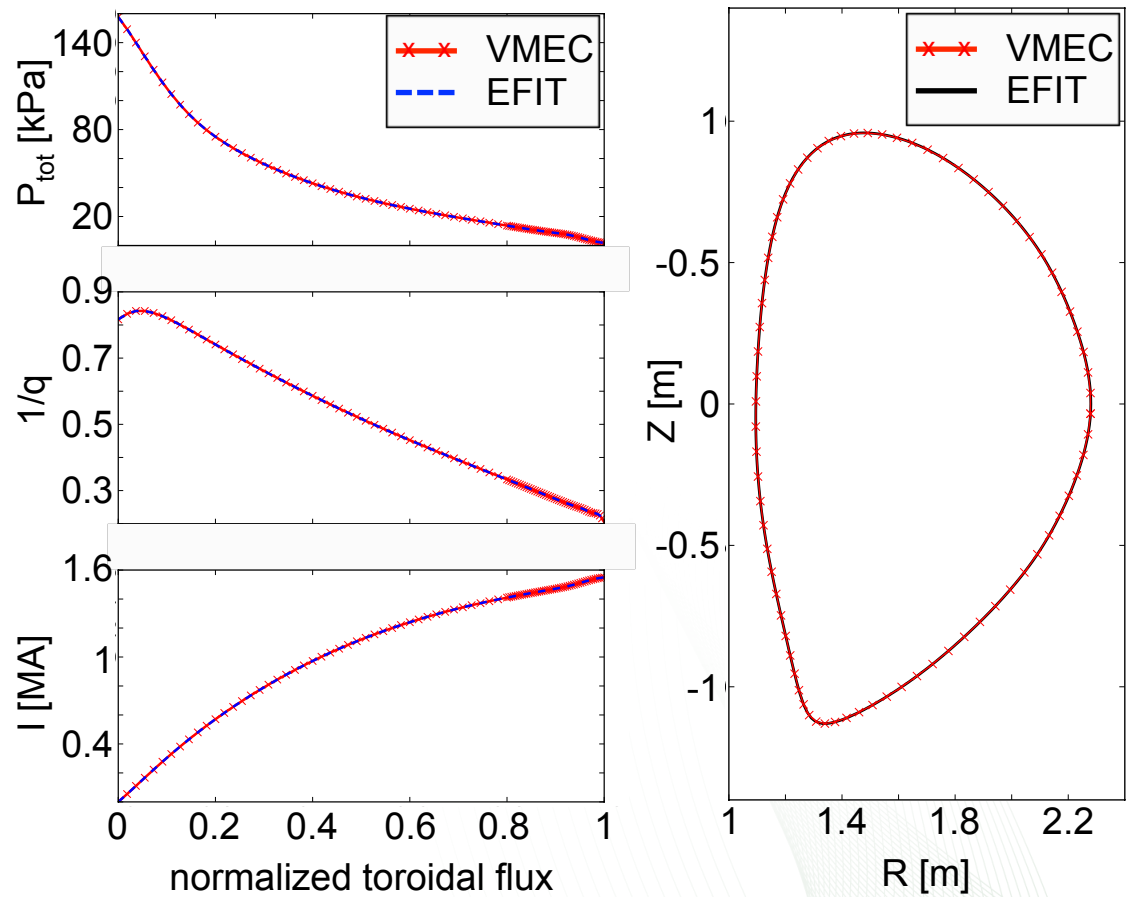
Use 2-D equilibrium as starting point → kinetic EFIT well developed and common

- **P_{tot}, 1/q, I profiles**
  - *use Akima splines*
  - *½ of points in the edge*
- **Poloidal Fourier modes of LCFS**
  - *minimized spectral power width*
- **Reads all currents from DIII-D MDS+ database**



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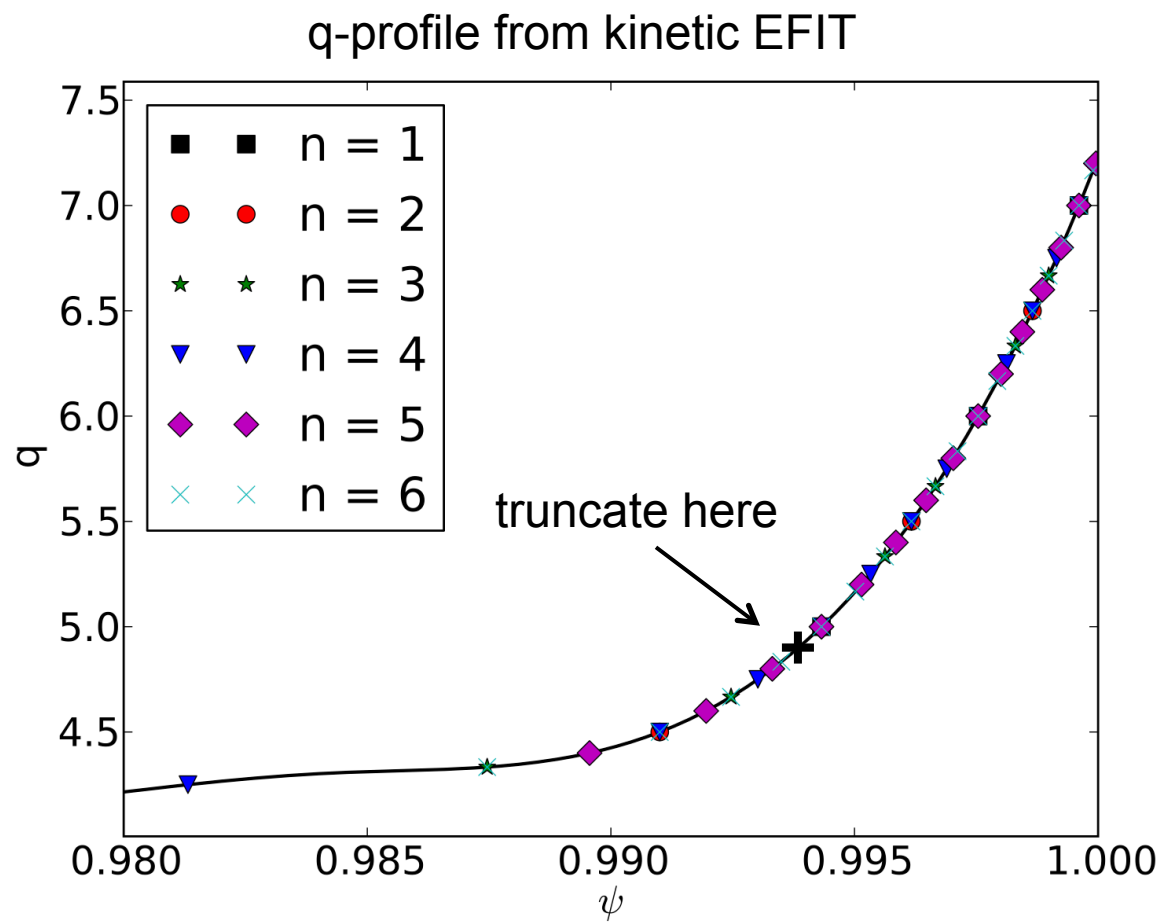
smart EFIT truncation essential to avoid numerical instabilities

- **Close to rational surface:**
  - *slow or no convergence*
  - *profiles oscillate at the edge*
  - *result changes with resolution*
- **Use gaps in rational surfaces**
  - *all above issues go away*



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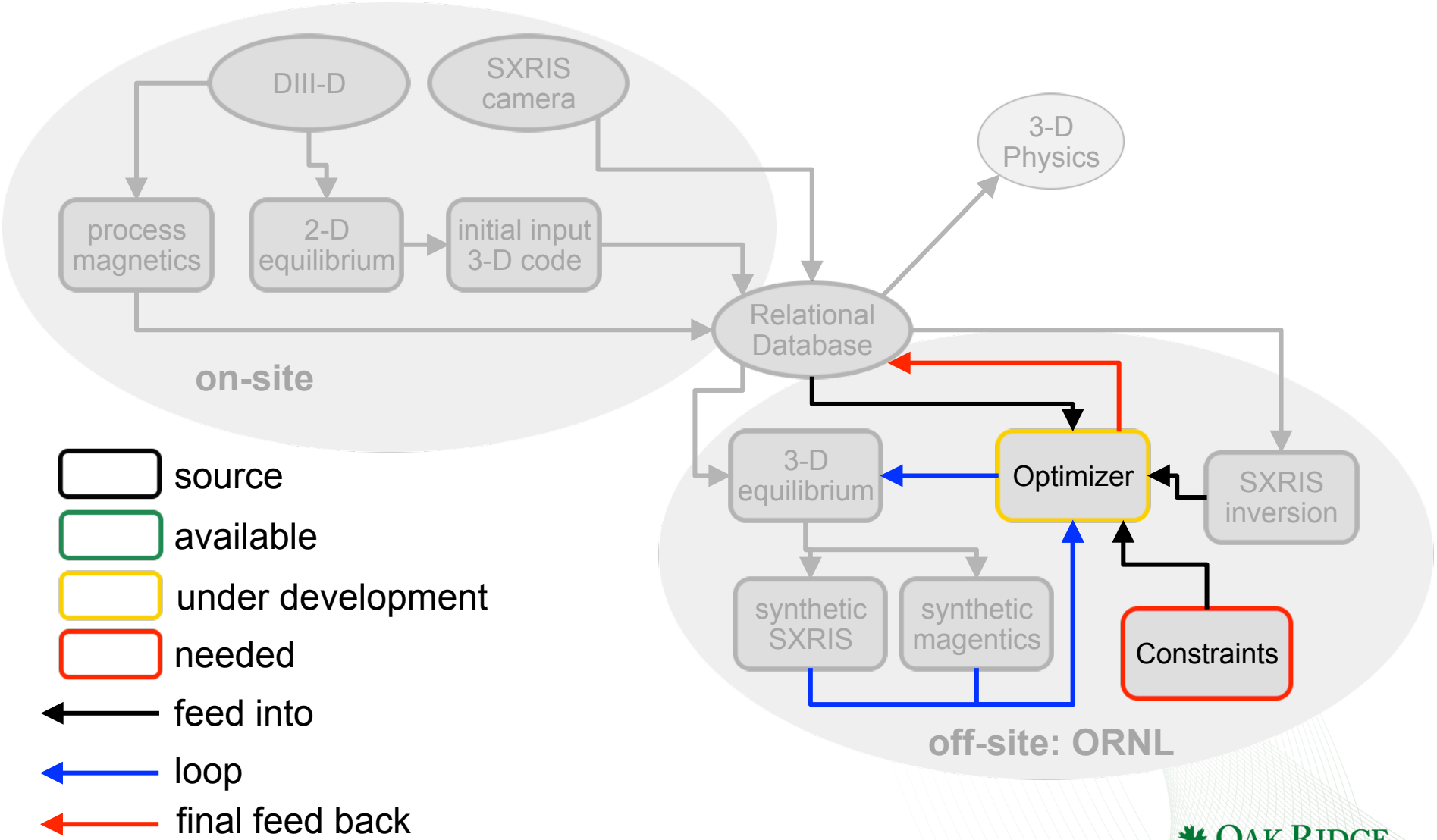
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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Optimizer allows feed -back/-forward

- **Reconstruction: compare 3-D measurements with synthetic signals, obtained from 3-D equilibrium → χ^2**
- **Modeling: compares synthetic 3-D signals with pre-defined constraints → χ^2**
- **Experiment at DIII-D**
  - *take data & reconstruct 3-D equilibrium*
  - *rerun code with pre-defined constraints*
    → identify how to run discharge differently
  - *redo experiment with predicted setup to test physics models*
- **Use & adapt V3FIT**

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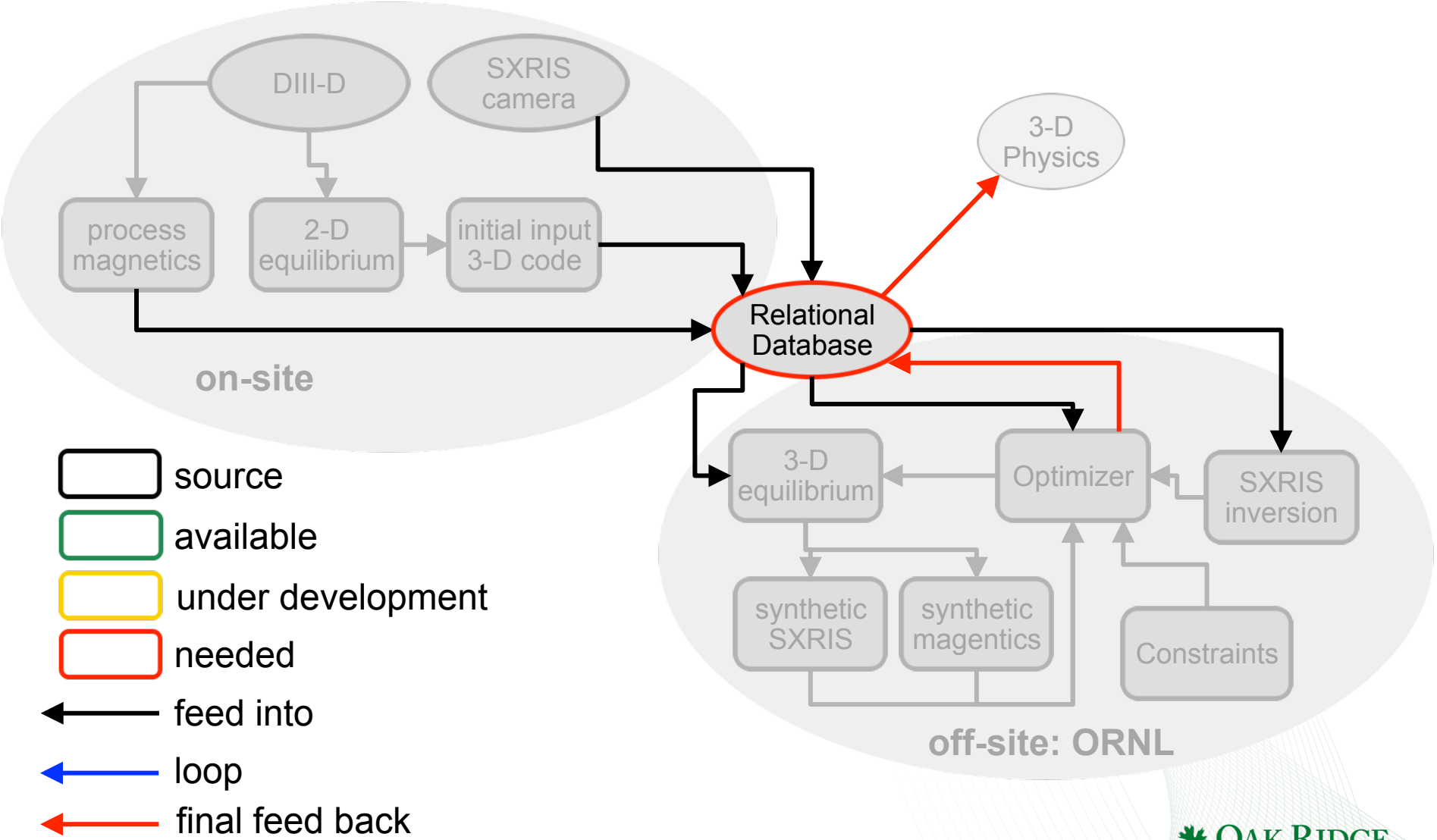
Workflow for 3-D reconstructions of H-mode DIII-D discharges



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A standardized Relational Database is a key missing element in fusion today

- **Stores and provides all input and output for further analysis & data integrety**
- **Combine MDS+ with SQL or NoSQL type relational database**
  - *no dublicate data → use pointer in MDS+*
  - *enable queries or data mining*
- **Efficiently transfers data between on- and off-site locations**
  - *sync MDS+ trees or bundle requests to minimize access time*
- **Project deliverable: Prototype for off-site collaboration with ITER?**

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Summary and Conclusions

- **Develop 3-D reconstruction**
  - *basis to test hypotheses for 3-D physics ELM suppression*
  - *today: one 3-D reconstruction could take weeks*
  - *future: in between shots? – like EFIT today*
- **Develop on-/off-site analysis toolset**
  - *implement relational database as a prototype for off-site collaboration in ITER era*
  - *today: up to ~3 GB/shot of data for 10 sec DIII-D shot*
  - *future: international devices (ITER) will have ~10-3000 times more data per shot: (100-3600 seconds pulses)*
- **Utilize ORNL's leadership class computational hardware & expertise**

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Year 1: Implementation of 3-D Toolset for On-/Off-site Computations

- **<u>Goal:</u> Determine, optimize, & test code-suite for analyzing 3-D, high-performance, tokamak physics at DIII-D**
  - *With off-site analysis & data transfer for rapidly available results*
- **<u>Focus/method:</u>**
  - *Implement enhanced 3-D reconstruction codes (e.g. parallelized)*
  - *Determine optimal diagnostic set*
    - *How many probes vs images vs profiles needed*
  - *Evaluate & develop pre-processing method*
  - *Do single 3-D reconstruction using toolset (not in "realtime")*

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Year 2: Couple the Analysis Code-suite to a Single DIII-D Experiment

- **<u>Goal:</u> Rapid turnaround (1 or 2 days) of 3-D equilibria of high-performance DIII-D discharges**
  - *Guide a DIII-D experimental run-day with proposed toolset*
  - *A paradigm of the expected ITER data-analysis environment*
- **<u>Focus/method:</u>**
  - *Development of scientific run-day to best utilize 3-D toolset*
  - *Deploy/test toolset for real-time feedback*
  - *Execute experimental run-day*

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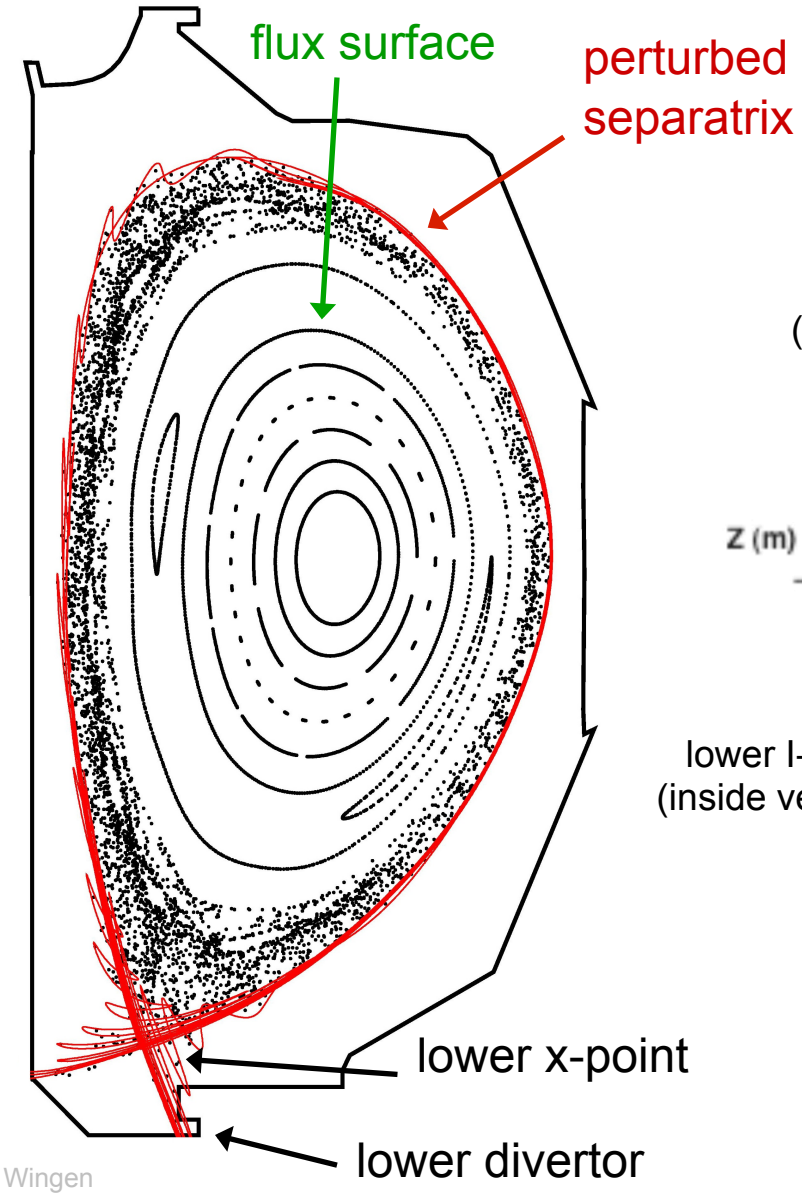
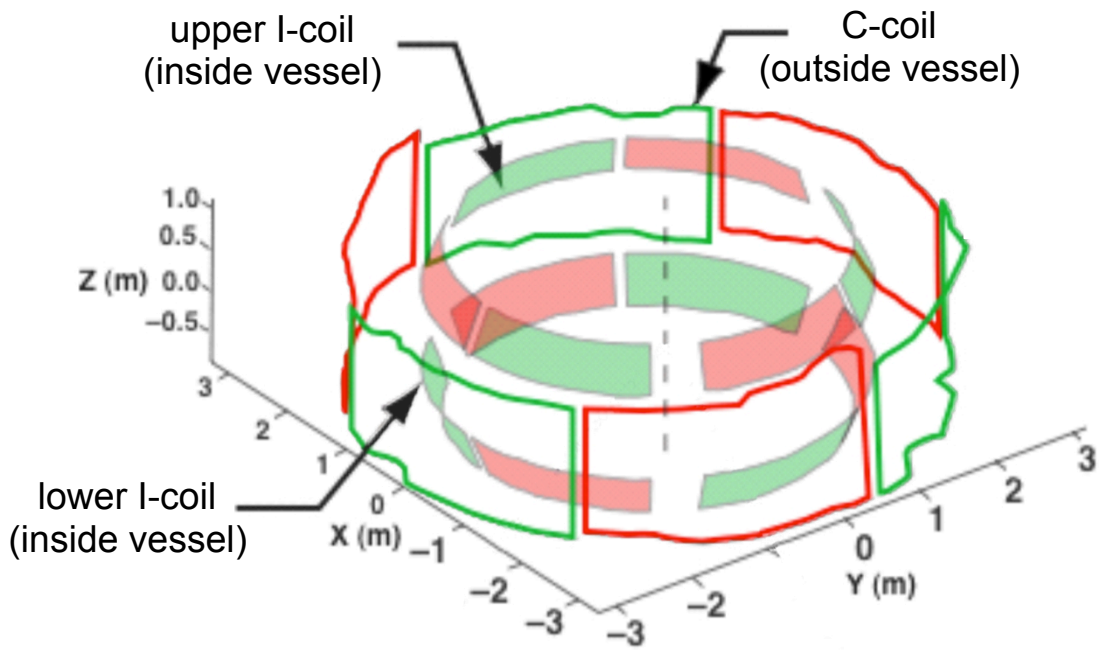
Backups

Vacuum approximation: 3D fields created by coils



Resonant Magnetic Perturbation (RMP) through applied fields



→ **large stochastic layer formation**

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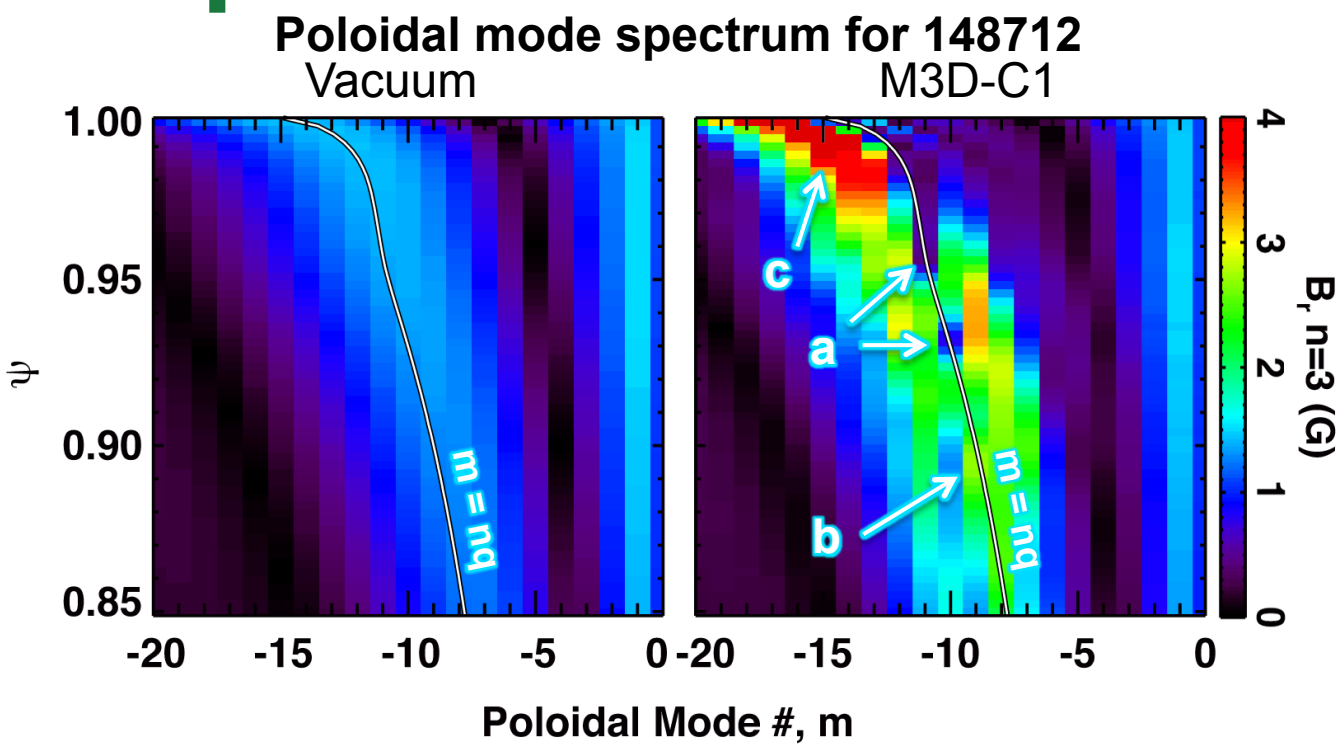
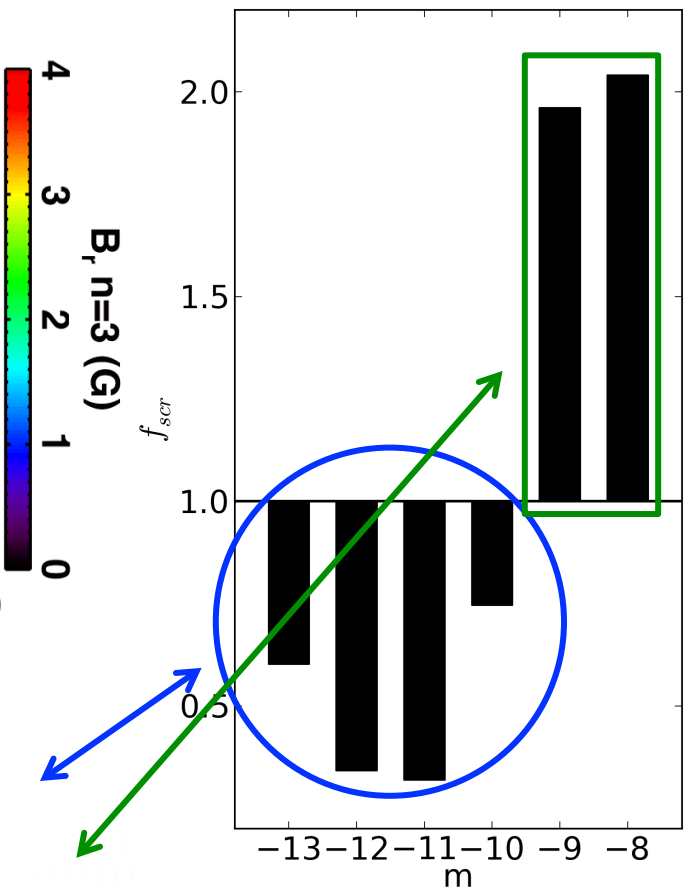
M3D-C1: linear, resistive, two-fluid MHD code calculates a plasma response to 3-D fields



$$f_{\rm scr} = B_{r,\rm pr}/B_{r,\rm vac}$$



Three main effects

- **a:** resonant screening → Islands shrink
- **b:** resonant amplification → Islands grow
- **c:** non-resonant amplification → kinking of flux surfaces

N.M. Ferraro, PoP **19**, 056105 (2012)

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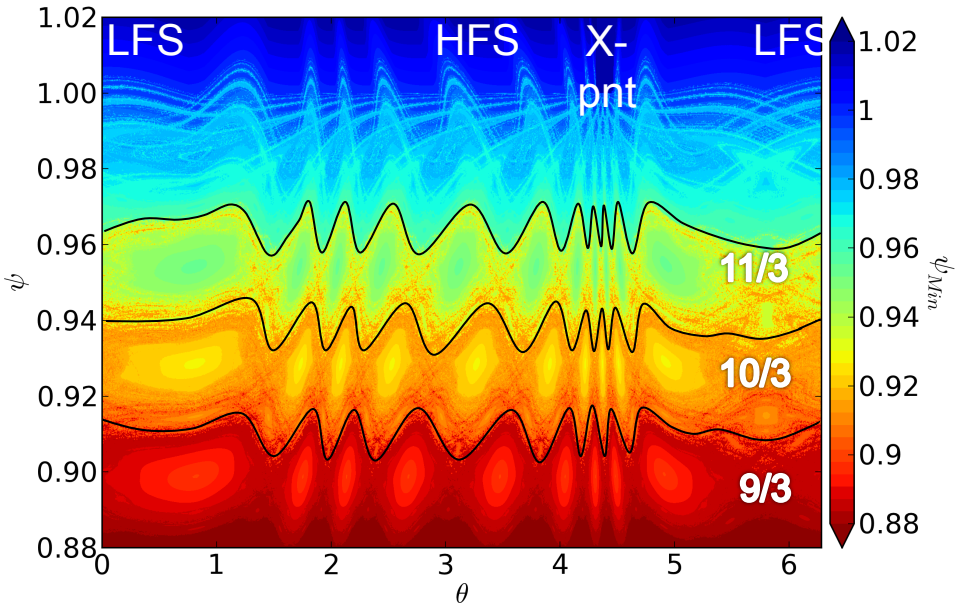
Plasma response significantly modifies magnetic topology: simulation shows all three effects

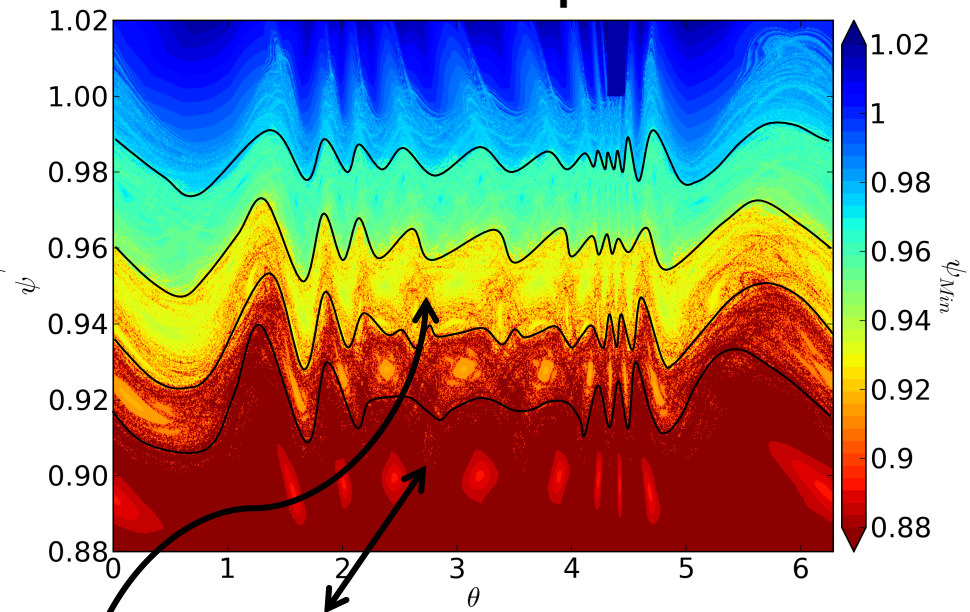
H-mode discharge with n = 3 RMP

Vacuum



color = penetration depth

Plasma Response



- island chains dominate structure
- stochastic regions → fractal
- radial phase inversion across islands

- **resonant amplification**, islands grow
- **resonant screening**, islands shrink
- **bended surfaces,** radially aligned → Kink response

Bending pushes islands away

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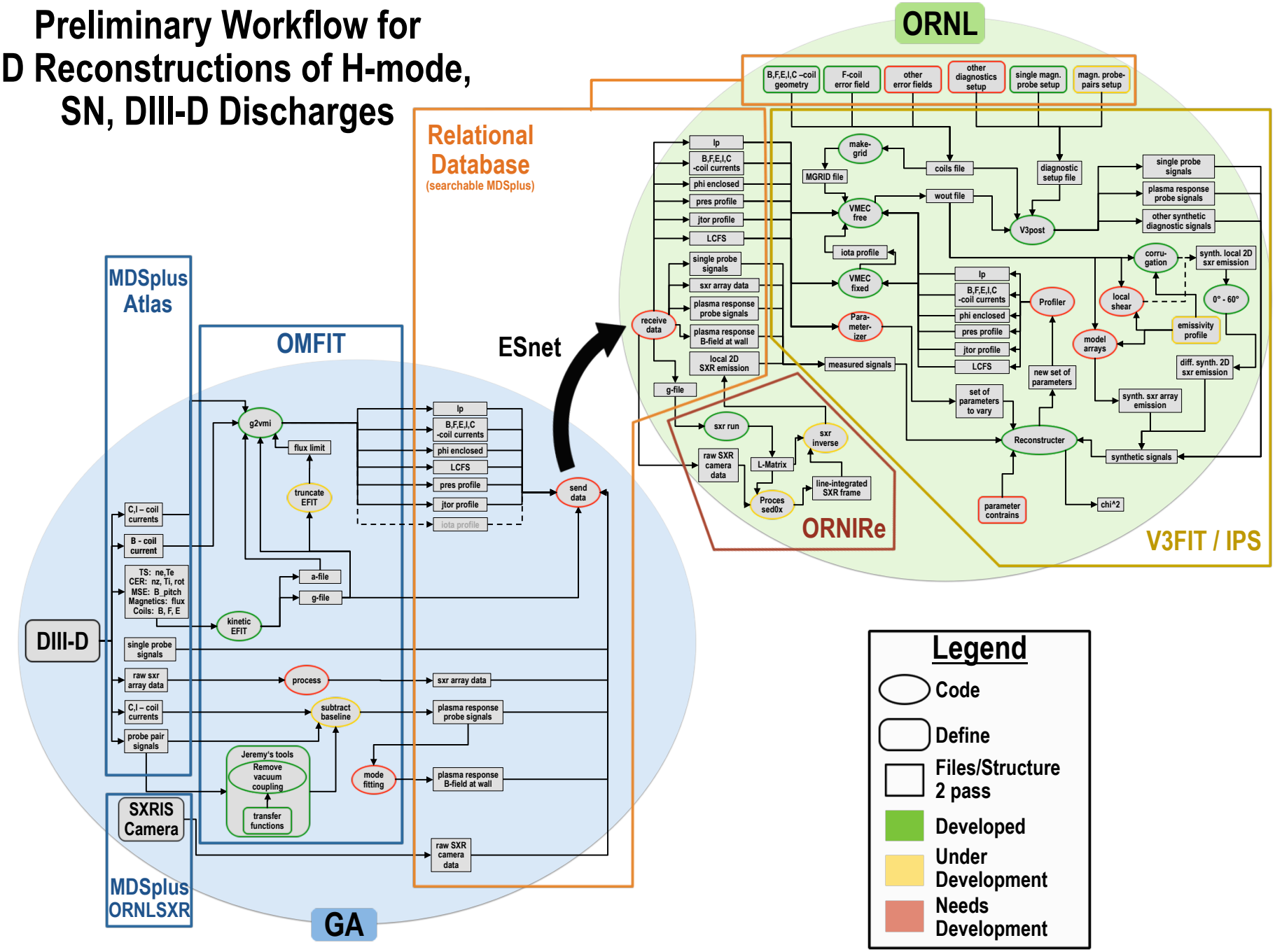
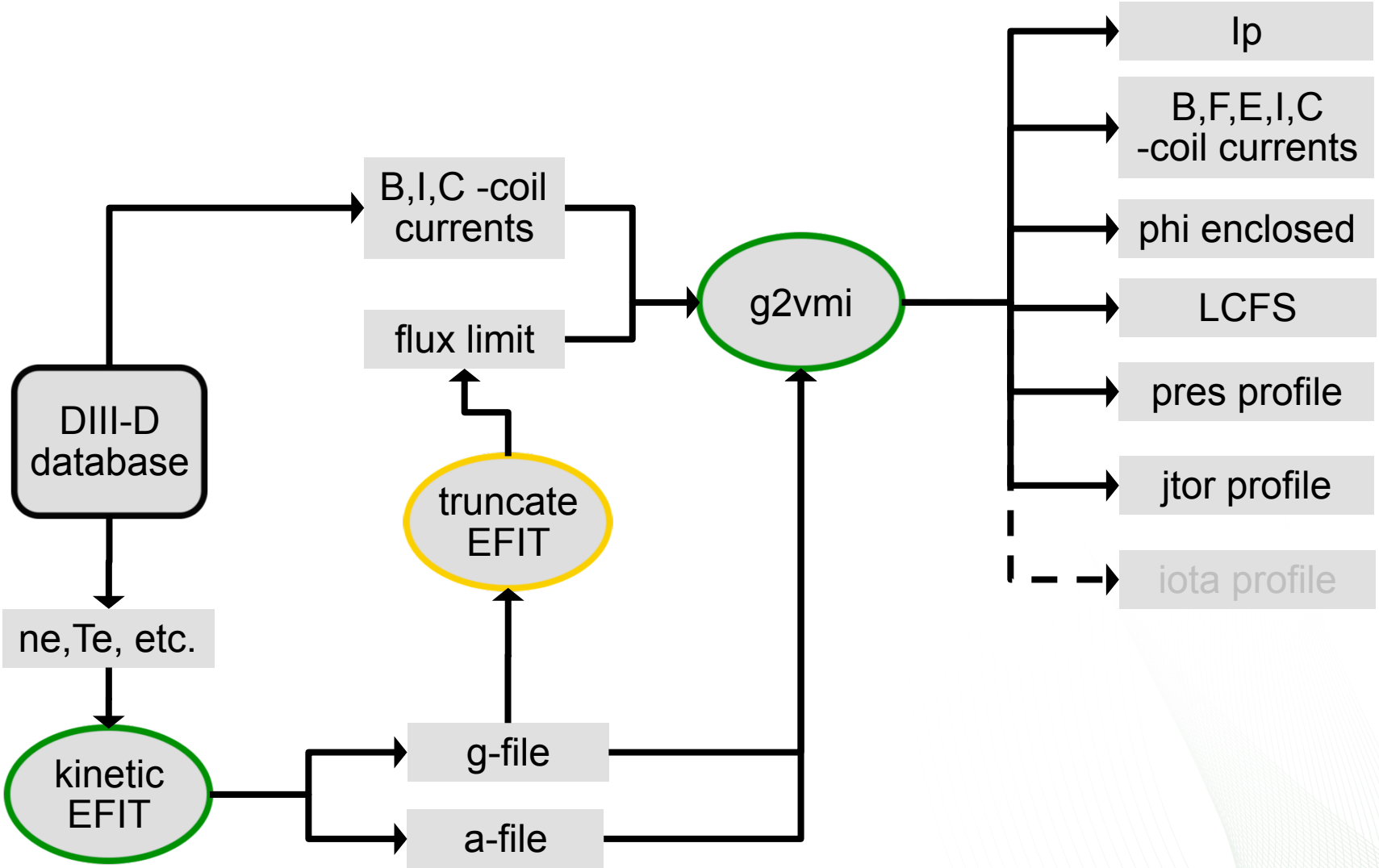
Preliminary Workflow for 3D Reconstructions of H-mode, SN, DIII-D Discharges



Prepare first 3D-equilibrium: g2vmi



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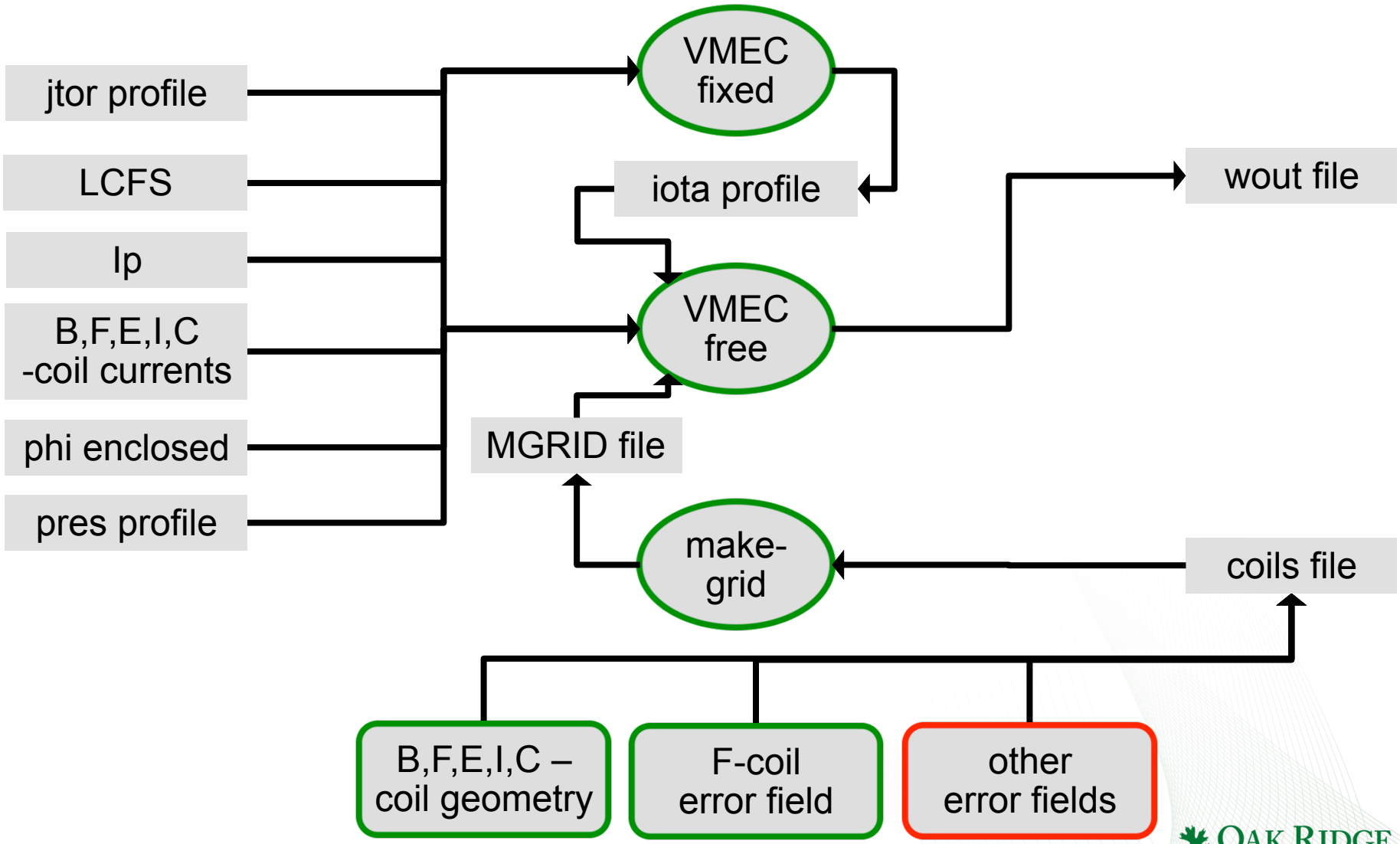
3D Equilibrium: VMEC



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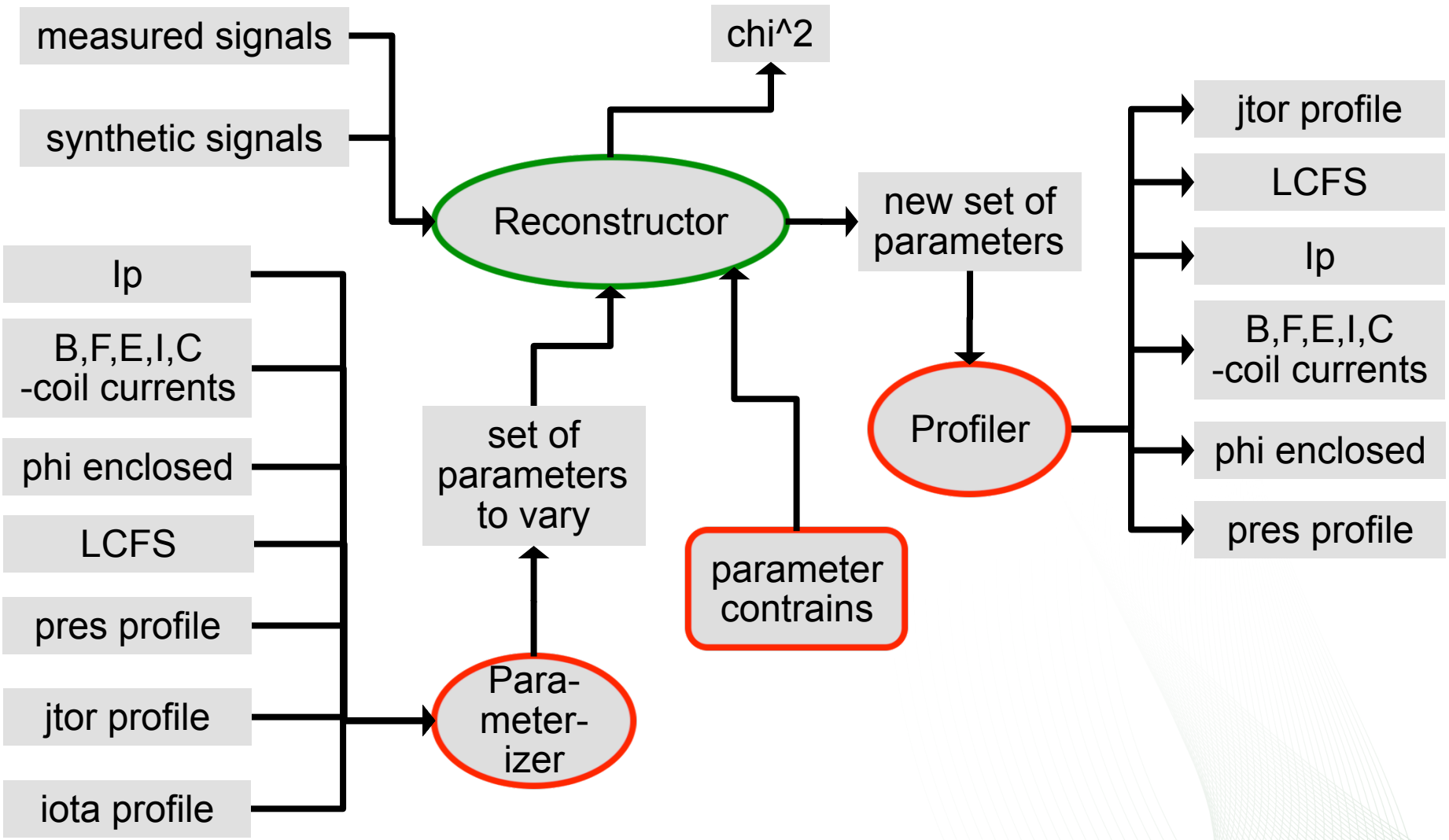
Optimizer, Reconstructor: Dakota, V3FIT



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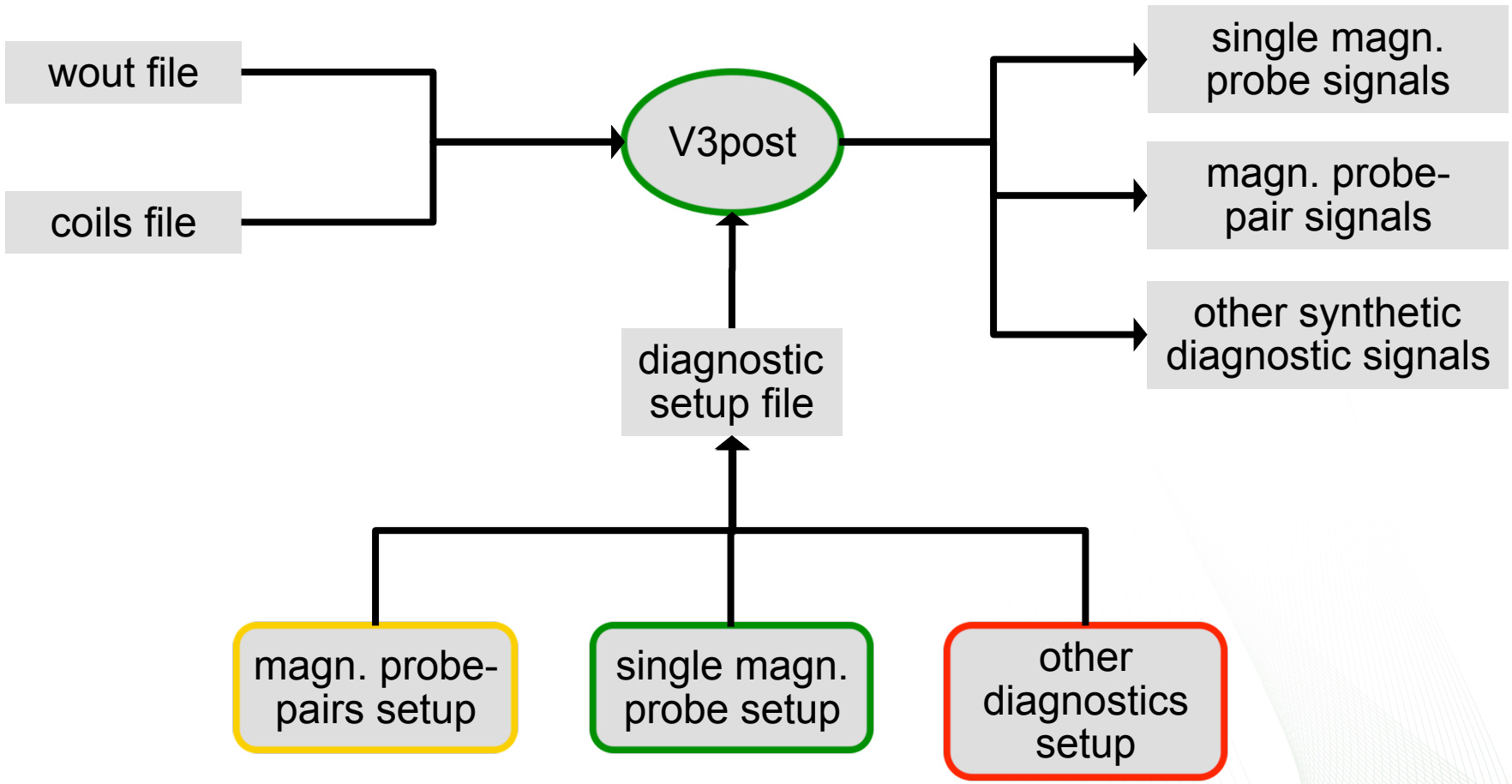
Synthetic measurements: V3post



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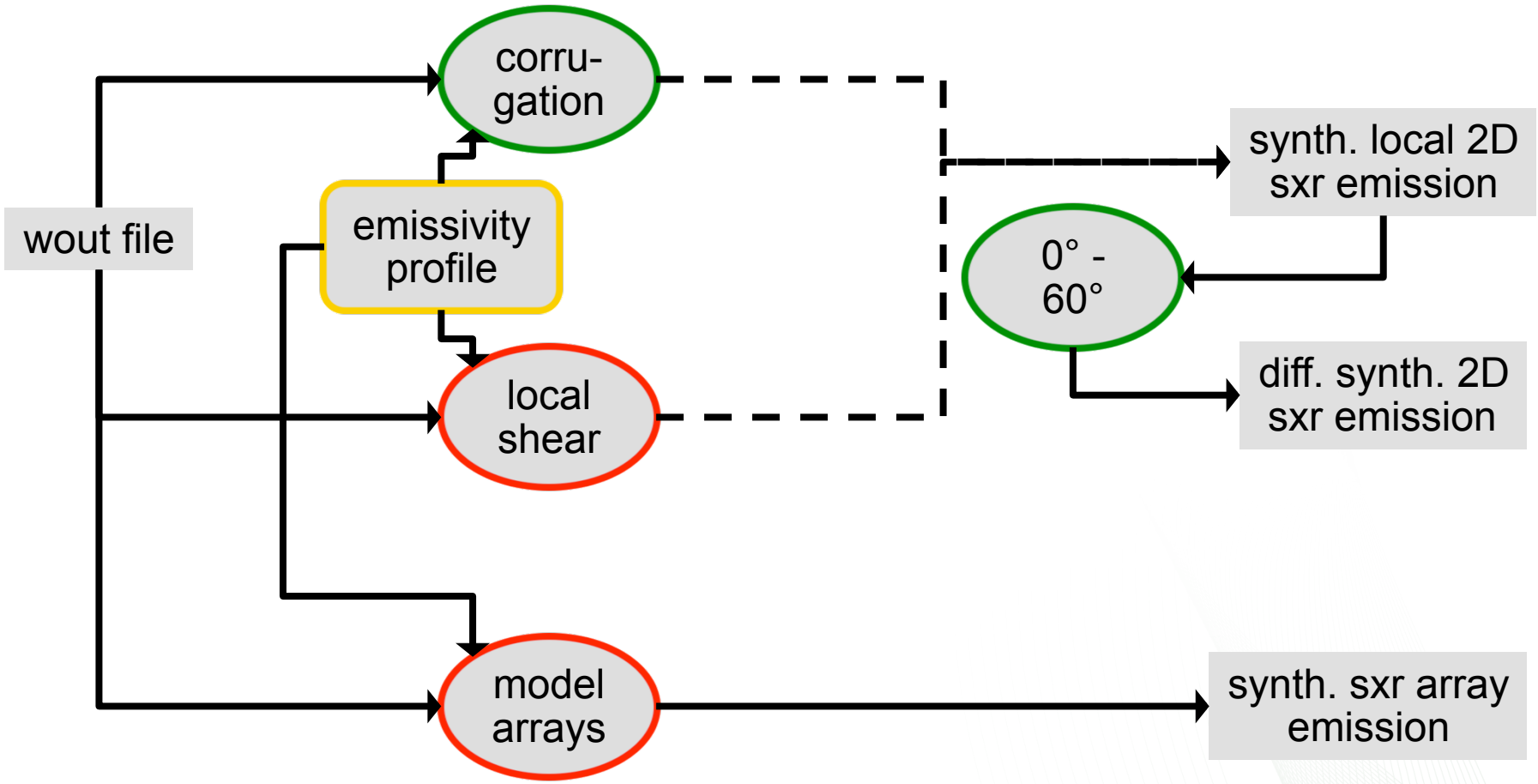
Synthetic SXR diagnostic



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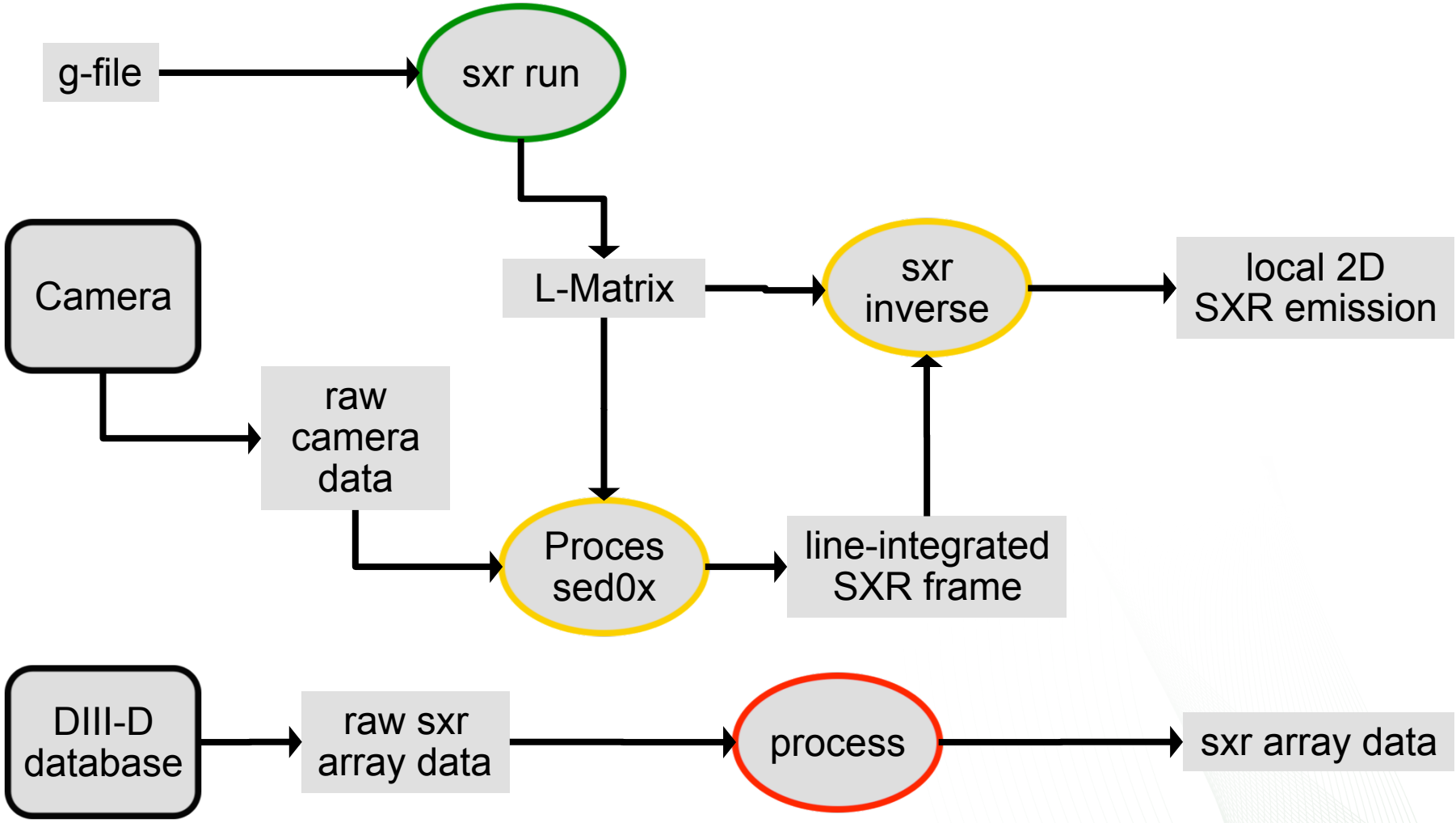
3D measurement postprocessing: SXR



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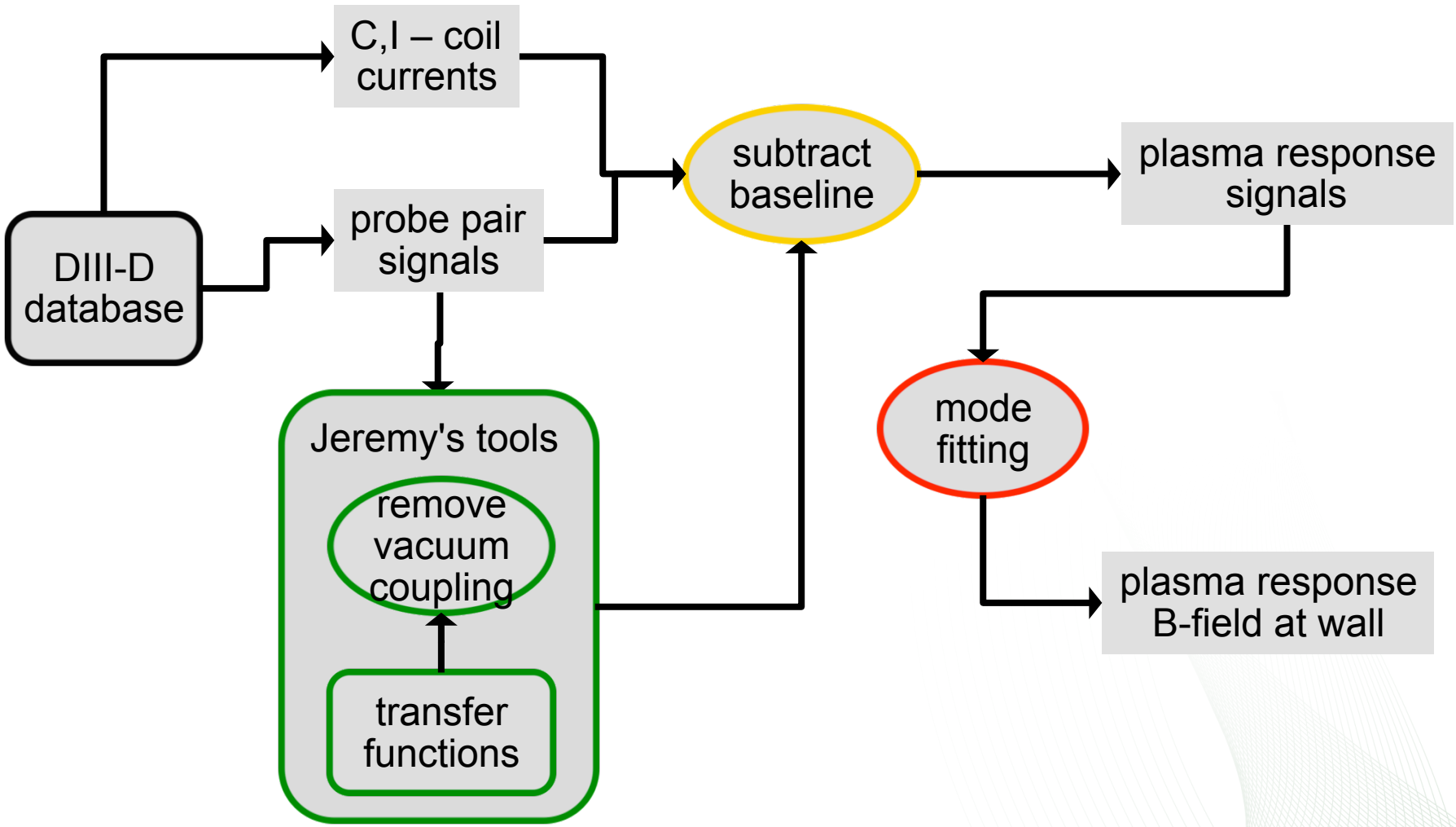
3D measurement postprocessing: probe pairs



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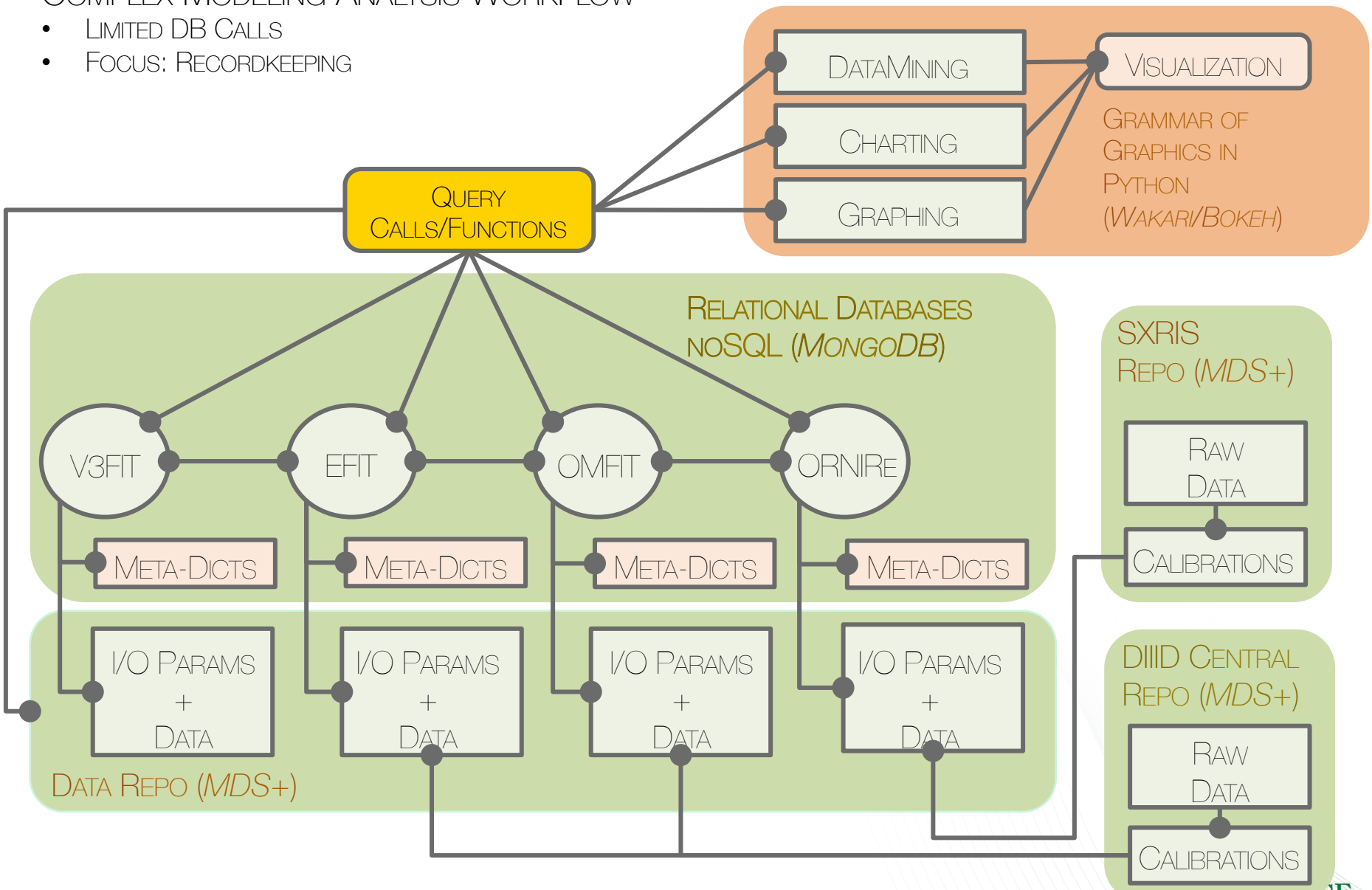
Complex Modeling Analysis WorkFlow

- Limited DB Calls
- Focus: Recordkeeping