A framework for the automated evaluation of two- and three-point correlation functions using distillation

John Bulava, for the Baryon Scattering Collabortion (BaSc)

Lattice2026, U. of Maryland, Jul. 27, 2026

Motivation:

- Distillation's benefit: computation of many correlators from few building blocks

- 'Physics' advantages:
  - Determination of excited states → scattering amplitudes

    Talk by H. Yan, M. Salg, M. Padmanath, A. Jackura, J. Stitson, S. Sharpe, J. Moscoso, J. Meneghini, J.-F. de la Garza
  - Improvement of ground state asymptotics

    Talks by J.-A. Urrea Nino, N. Mathur, A. Stump

- 'Implementation' advantages:
  - Automation
  - Tensor contraction is a well-known problem

- This Talk: details of our implementation

History of distillation: (personal viewpoint)

- Original Paper: M. Peardon, et al., Phys.Rev.D 80 (2009) 054506

  → V^2 scaling

- Early adopters:
  - Hadron Spectrum Collaboration

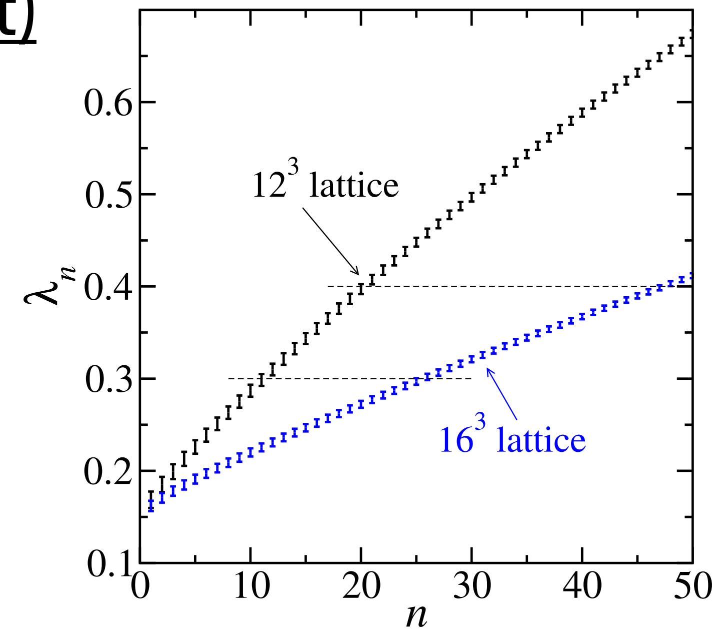
    J. Dudek, et al., Phys.Rev.Lett. 103 (2009) 262001
    JB, et al., Phys.Rev.D 82 (2010) 014507
    J. Dudek et al., Phys.Rev.D 83 (2011) 071504

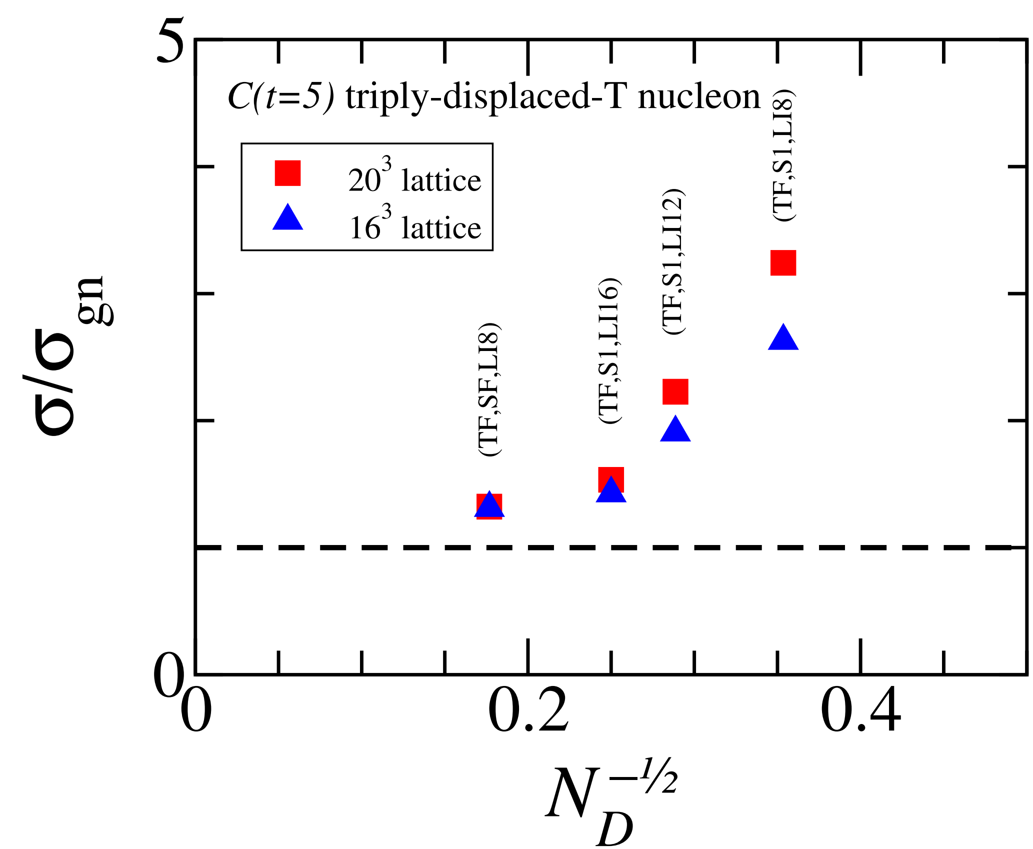
  - Graz-Ljubljana group

    C. B. Lang, et al., Phys.Rev.D 84 (2011) 5, 054503

- Stochastic-LapH:

  C. Morningstar, et al., Phys.Rev.D 83 (2011) 114505
  - Noise+dilution in the LapH subspace
  - Volume scaling improved





History of distillation:

- Downside of Stoch. Laph: independent estimators for each quark line

- Upside of distillation: GPU's help

- My current viewpoint:
  - Full distillation for the perambulators
  - Stochastic estimators (if needed) for correlator construction

- Software for automated correlator computation:
  - OpPy: Group-theoretical operator construction
  - PyWick: enumeration of Wick contractions
  - QudaLaph: computation of tensors
  - PyCorr: construction of correlators

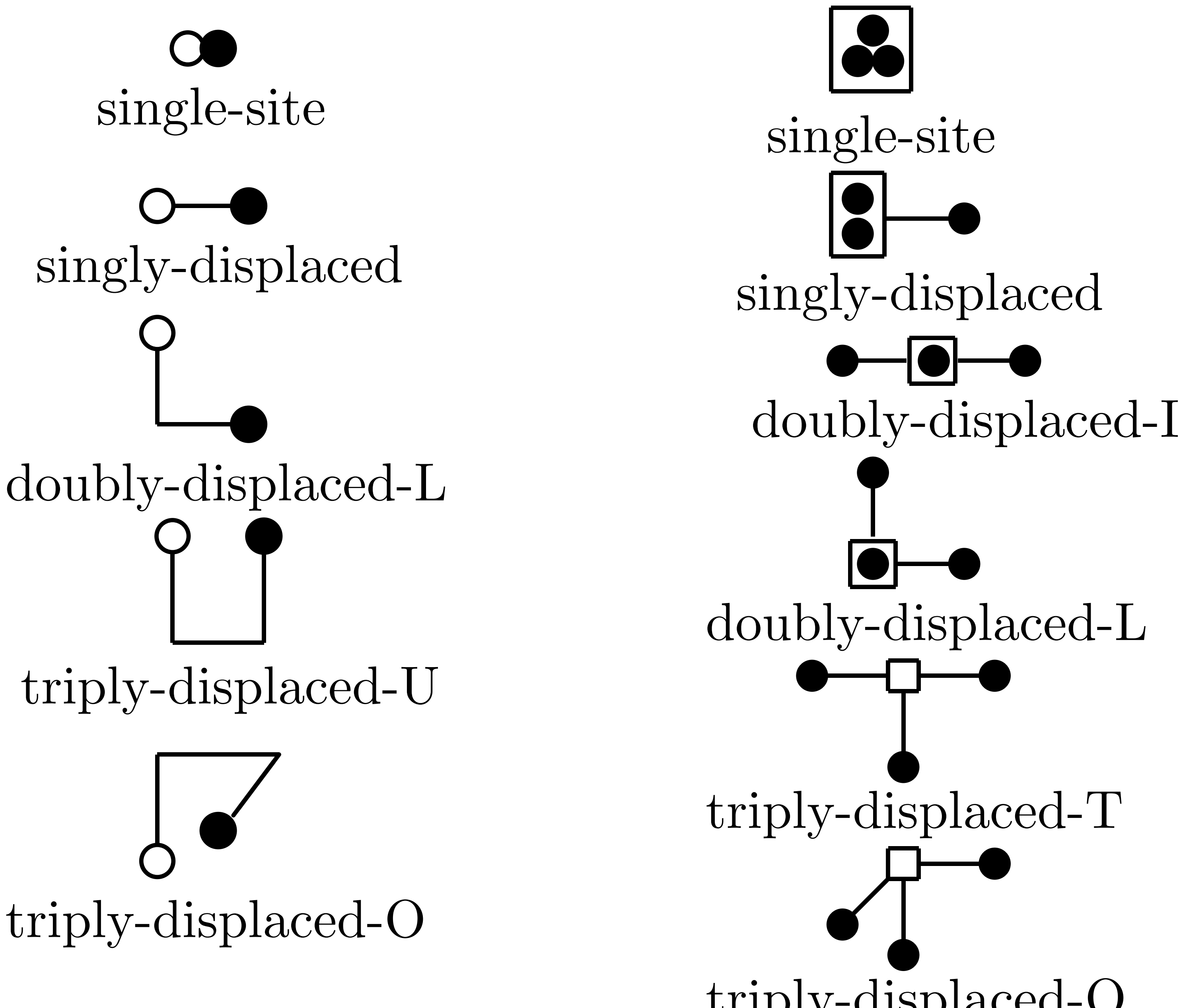
  (Very much under construction!)

- See also:
  - Redstar J. Chen, et al., Proceedings of PASC2023
  - OpTion H. Yan, et al., JHEP 10 (2025) 210

Operator Wishlist: single-hadron operators

S. Basak, et al., Phys.Rev.D 72 (2005) 094506

Meson configurations	Baryon configurations



OpPy:

S. Reibert, JB, in prep.

- Previous baryon work: automated projection for each type, momenta

  S. Basak, et al., Phys.Rev.D 72 (2005) 094506

  - Lacks insight into nature of the operators

- Clebsch-Gordan combination of spins+displacements

  S. Basak, et al., Phys.Rev.D 72 (2005) 074501
  J. Dudek, et al., Phys.Rev.D 82 (2010) 034508

$$\Lambda_{\text{spin}} \otimes \Lambda_{\text{disp}} = \Lambda_{\text{tot}}$$

- Factorization enabled by symmetrization:

$${}^{\Lambda}B^{D}_{\alpha\beta\gamma}(\boldsymbol{x}) = \sum_{\sigma \in S_{\text{p}}} \gamma^{\Lambda}(\sigma) B^{\sigma(D)}_{\alpha\beta\gamma}$$

- Exhaustive classification of flavor symmetries

- Subduction onto moving irreps

- CG series for multi-hadron operators

  N. Blume, S. Reibert, JB, in prep
  See also: W. Detmold, et al., Phys.Rev.D 109 (2024) 9, 094516

Baryon	Operator	Symmetry Class
Δ^{++}	uuu	S_{3+}
Σ^{+}	uus	Σ_{1+}
	usu	Σ_{2+}
	suu	Σ_{3+}
N^{+}	$udu - duu$	Σ^{*}_{1-}
	$uud - duu$	Σ^{*}_{2-}
	$uud - udu$	Σ^{*}_{3-}
Λ^{0}	$uds - dus$	Σ_{1-}
	$usd - dsu$	Σ_{2-}
	$sud - sdu$	Σ_{3-}

OpPy:

- Symmetrization of flavor:
  - nucleon operators:

$$N_{+1/2} = d^{N}_{\alpha\beta\gamma}\left(\Phi^{uud}_{\alpha\beta\gamma} - \Phi^{duu}_{\alpha\beta\gamma}\right)$$
$$N_{-1/2} = d^{N}_{\alpha\beta\gamma}\left(\Phi^{udd}_{\alpha\beta\gamma} - \Phi^{ddu}_{\alpha\beta\gamma}\right)$$

  - demand operator coefficients satisfy:

$$d^{N}_{\alpha\beta\gamma} = d^{N}_{\beta\alpha\gamma}, \qquad d^{N}_{\gamma\beta\alpha} + d^{N}_{\alpha\gamma\beta} = -d^{N}_{\alpha\beta\gamma}$$

  - now operators expressed as:

$$N_{+1/2} = d^{N}_{\alpha\beta\gamma}\Phi^{uud}_{\alpha\beta\gamma}$$
$$N_{-1/2} = -d^{N}_{\alpha\beta\gamma}\Phi^{ddu}_{\alpha\beta\gamma}$$

  - Reduction in the number of Wick contractions

PyWick: automated enumeration of Wick contractions

H. Alharazin, F. Alvarado, JB, D. Laudicina, F. Romero-Lopez, M. Salg in prep.
see also: D. Djukanovic, Comput.Phys.Commun. 247 (2020) 106950
A. Hackl, C. Lehner, Phys.Rev.D 113 (2026) 11, 114502

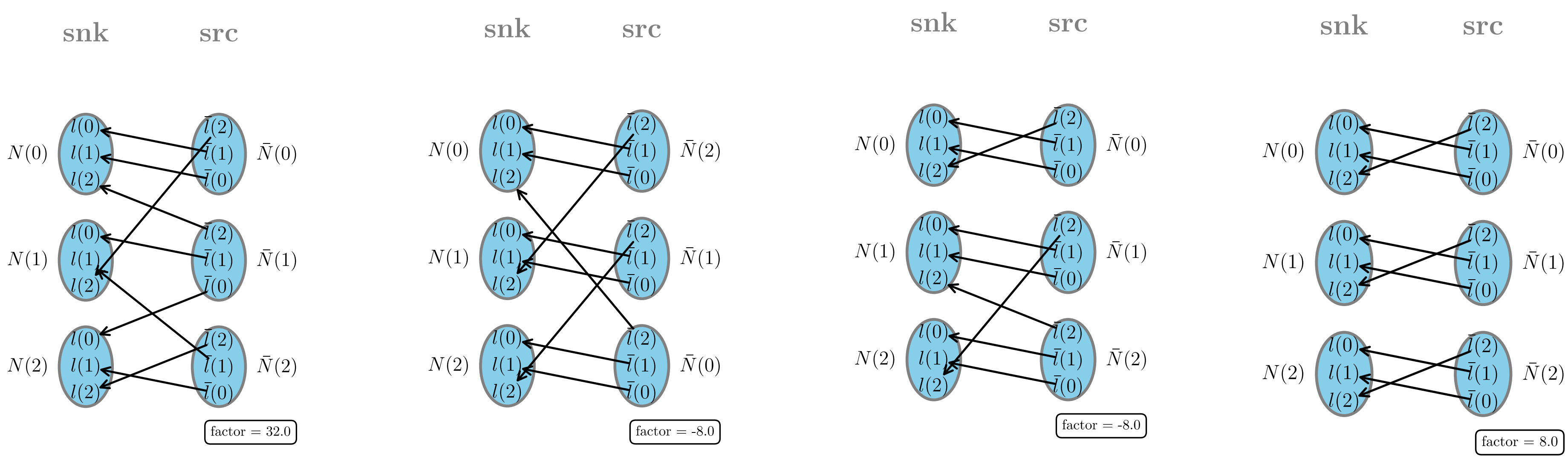
- Wick contraction encoded as integer array of quark lines :

  [[[1, 0, 0], [0, 0, 1]], [[1, 0, 1], [0, 0, 0]], [[1, 0, 2], [0, 0, 2]]]

- Each quark line has format

  [[tf, hadron_f, quark_f], [t0, hadron_0, quark_0]]

- States included:
  - Single hadrons
  - SU(2) and SU(3) multi-hadron multiplets (up to 3 hadrons)
- Baryon index symmetries are important!
  - Ex: 3n → 3n: 4320 diagrams → 126 diagrams



QudaLaph: background

M. Peardon, et al., Phys.Rev.D 80 (2009) 054506

- Laplacian-Heaviside (LapH) quark smearing:

$$S_{ab}(\boldsymbol{x},\boldsymbol{x}') = \Theta(\sigma_{\mathrm{s}}^2 + \Delta) \approx \sum_{k=1}^{N_{\mathrm{ev}}} v_a^{(k)}(\boldsymbol{x})\, v_b^{(k)}(\boldsymbol{x}')^*$$

- Factorization of smeared quark propagator:

$$Q_f(a,\alpha,\boldsymbol{y},t|b,\beta,\boldsymbol{x},t_0) = \sum_{k,k'=1}^{N_{\mathrm{ev}}} v_a^{(k)}(\boldsymbol{y},t) \times$$
$$P_f(k,\alpha,t|k',\beta,t_0)\, v_b^{(k')}(\boldsymbol{x},t_0)^*$$

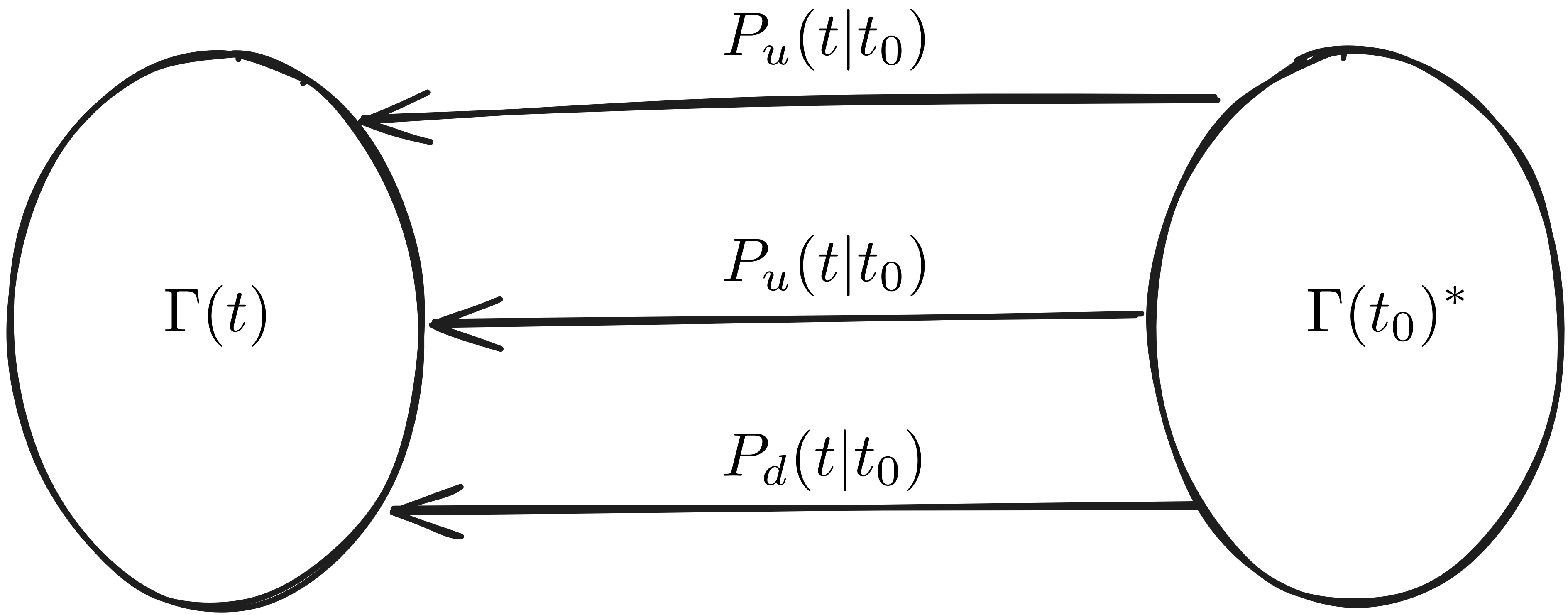
QudaLaph: background

Correlators constructed from several tensors:

- **Perambulator:**

$$P_f(k,\alpha,t|k',\beta,t_0) = \sum_{a,b}\sum_{\boldsymbol{x},\boldsymbol{y}} v_a^{(k)}(\boldsymbol{x},t)^* \times$$
$$Q_f(a,\alpha,\boldsymbol{x},t|b,\beta,\boldsymbol{y},t_0)\, v_b^{(k')}(\boldsymbol{y},t_0)$$

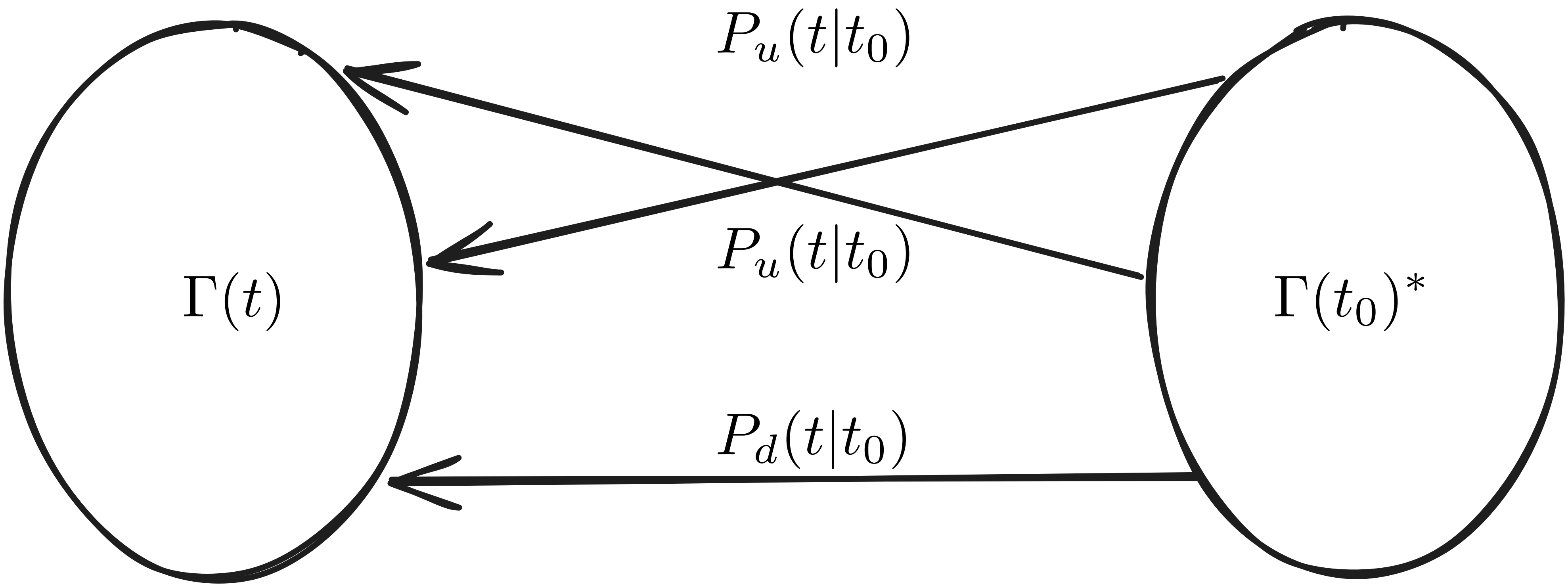
Correlator construction: baryon



Mode triplet:

$$\Gamma_{ijk}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} \mathrm{e}^{i\boldsymbol{p}\cdot\boldsymbol{x}}\,\epsilon_{abc}\,v_a^{(i)}(\boldsymbol{x},t)\,v_b^{(j)}(\boldsymbol{x},t)\,v_c^{(k)}(\boldsymbol{x},t)$$

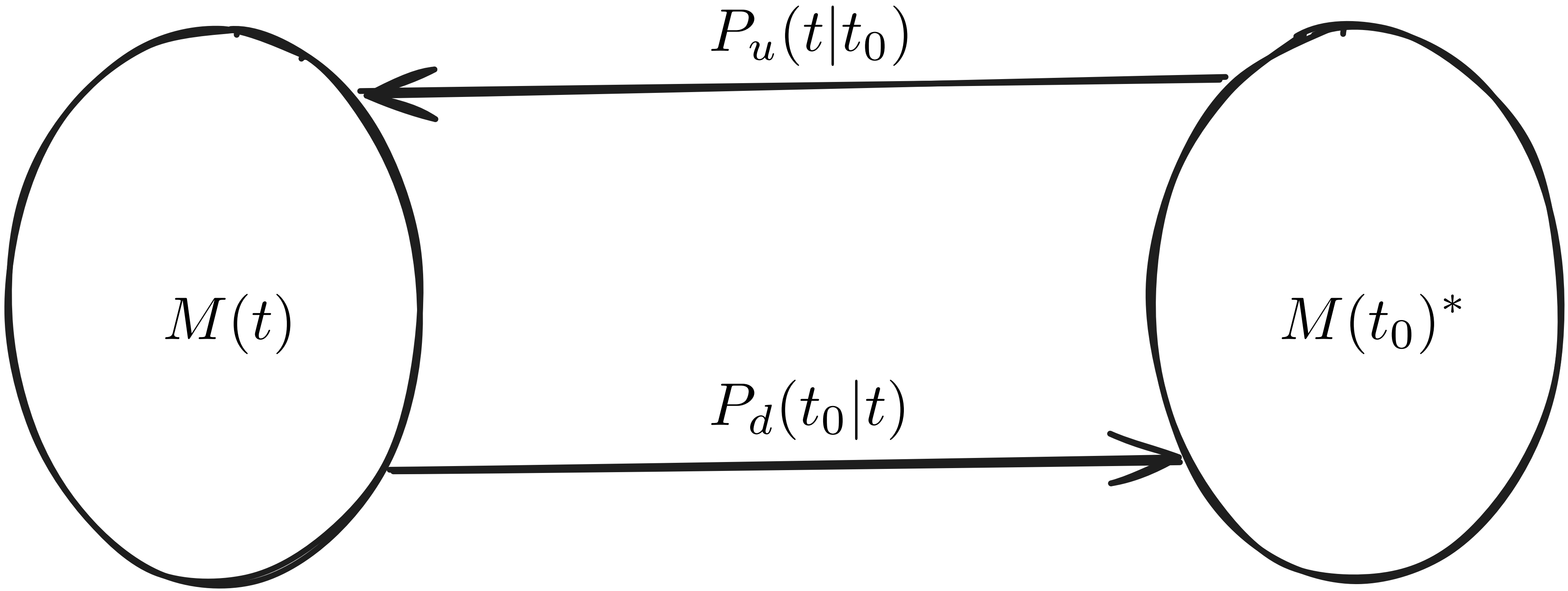
Correlator construction: baryon



Mode triplet:

$$\Gamma_{ijk}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} \mathrm{e}^{i\boldsymbol{p}\cdot\boldsymbol{x}}\, \epsilon_{abc}\, v_a^{(i)}(\boldsymbol{x},t)\, v_b^{(j)}(\boldsymbol{x},t)\, v_c^{(k)}(\boldsymbol{x},t)$$

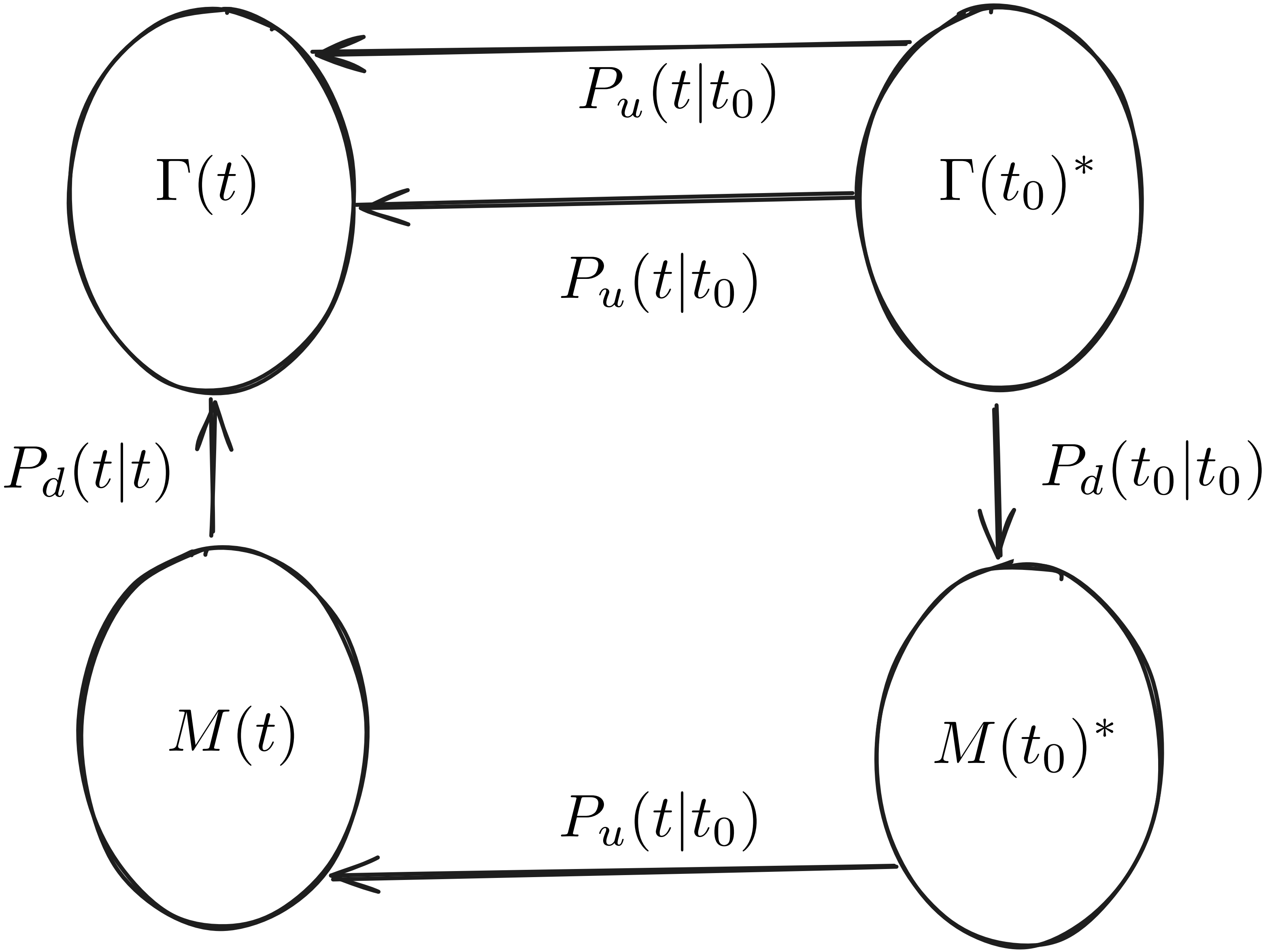
Correlator construction: meson



Mode doublet:

$$M_{ij}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} \mathrm{e}^{i\boldsymbol{p}\cdot\boldsymbol{x}}\,\delta_{ab}\,v_a^{(i)*}(\boldsymbol{x},t)\,v_b^{(j)}(\boldsymbol{x},t)$$

Correlator construction: meson-baryon



- Same-time perambulators required

QudaLapH:

C. Morningstar, J. Hudspith, K. Clark

- Compute perambulators, mode doublets, mode triplets on GPU's
- Current status: Perambulators fully supported
- All computations performed on GPUs:
  - Gauge field smearing
  - Eigenvector computation
  - Dirac matrix inversion
  - LapH subspace projection
- Publicly available: here

PyCorr:

H. Alharazin, JB, D. Laudicina, C. Morningstar, F. Romero-Lopez, M. Salg, in prep.

- Contract tensors from QudaLaph, using PyWick and OpPy
- ElementalGraph:
  - Fully connected sub-diagram of a Wick contraction
  - Single hadron elemental for each hadron: HadronElementalInfo
  - All required combinations of elementals stacked for batched evaluation
- Three Stages:
  - Setup (CPU): for a list of correlators, determine all ElementalGraphs
  - Compute (GPU): do the contractions
  - Project (CPU): linear combinations of (products of) ElementalGraphs

PyCorr:

H. Alharazin, L. Barca, JB, D. Laudicina, C. Morningstar, F. Romero-Lopez, M. Salg, in prep.

- Example: Nucleon channel at rest (I=1/2, B=1, G1g) on CLS X252

$$N_{\rm f} = 2+1,\ m_\pi = 280{\rm MeV},\ 36^3 \times 128,\ N_{\rm cfg} = 26,\ N_{t_0} = 16$$

```
nucleon_psq0_g1g = [
 [['N',0]],     ← [hadron_name, psq]
[['Nstar',0]],
[['f0',0],['N',0]],
[['pi',1],['N',1]],
[['eta',1],['N',1]],
[['pi',1],['D',1]],
[['pi',0],['pi',0],['N',0]],
]
```

- Output of Setup step: 375 ElementalGraphs, stack sizes ~ 10-10,000

- Compute step: 300sec per source time on single NVIDIA A30

PyCorr:

H. Alharazin, L. Barca, JB, D. Laudicina, C. Morningstar, F. Romero-Lopez, M. Salg, in prep.
See also: A. Hackl and C. Lehner, Phys.Rev.D 113 (2026) 11, 114502

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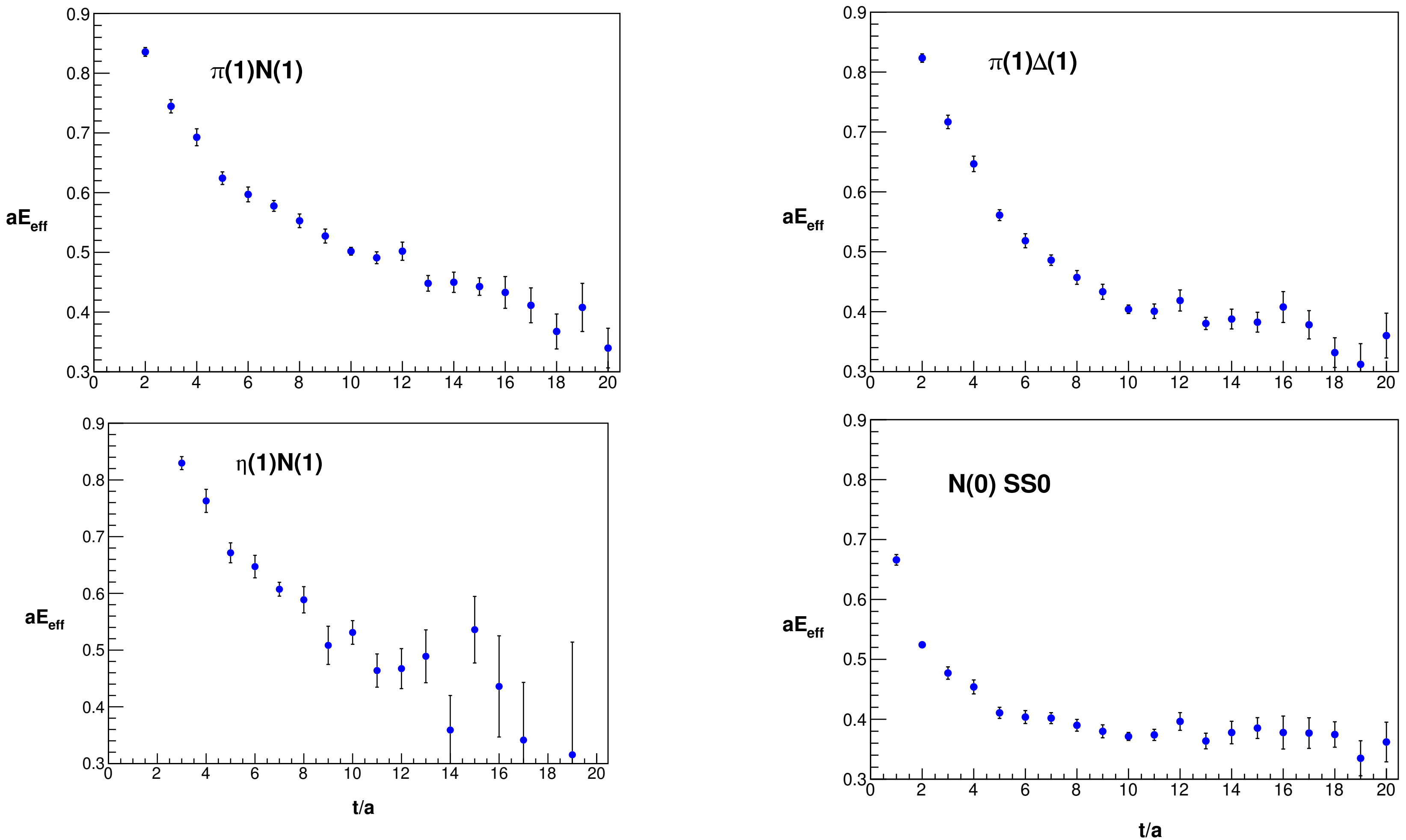
- Results: diagonal effective masses (preliminary)



PyCorr:

H. Alharazin, L. Barca, JB, D. Laudicina, C. Morningstar, F. Romero-Lopez, M. Salg, in prep.
See also: H. Yan, et al., Phys.Rev.Lett. 133 (2024) 21, 211906

- Example: Omega at rest (I=0, T1um)

$$N_{\mathrm{f}} = 2+1,\ m_\pi = 280\mathrm{MeV},\ 36^3 \times 128,\ N_{\mathrm{cfg}} = 350,\ N_{t_0} = 4$$

```
omega_psq0_t1u = [
[['omega',0]],
[['phi',0]],
[['pi',1],['rho',1]],
[['K',1],['Kbar',1]]
]
```

- Two each of omega, phi, and rho operators → Nop = 7
- Output of Setup step: 15 ElementalGraphs, stack sizes up to ~100,000
- First three pion state: [['pi',1],['pi',1],['pi',2]] (high lying)

PyCorr:

H. Alharazin, L. Barca, JB, D. Laudicina, C. Morningstar, F. Romero-Lopez, M. Salg, in prep.

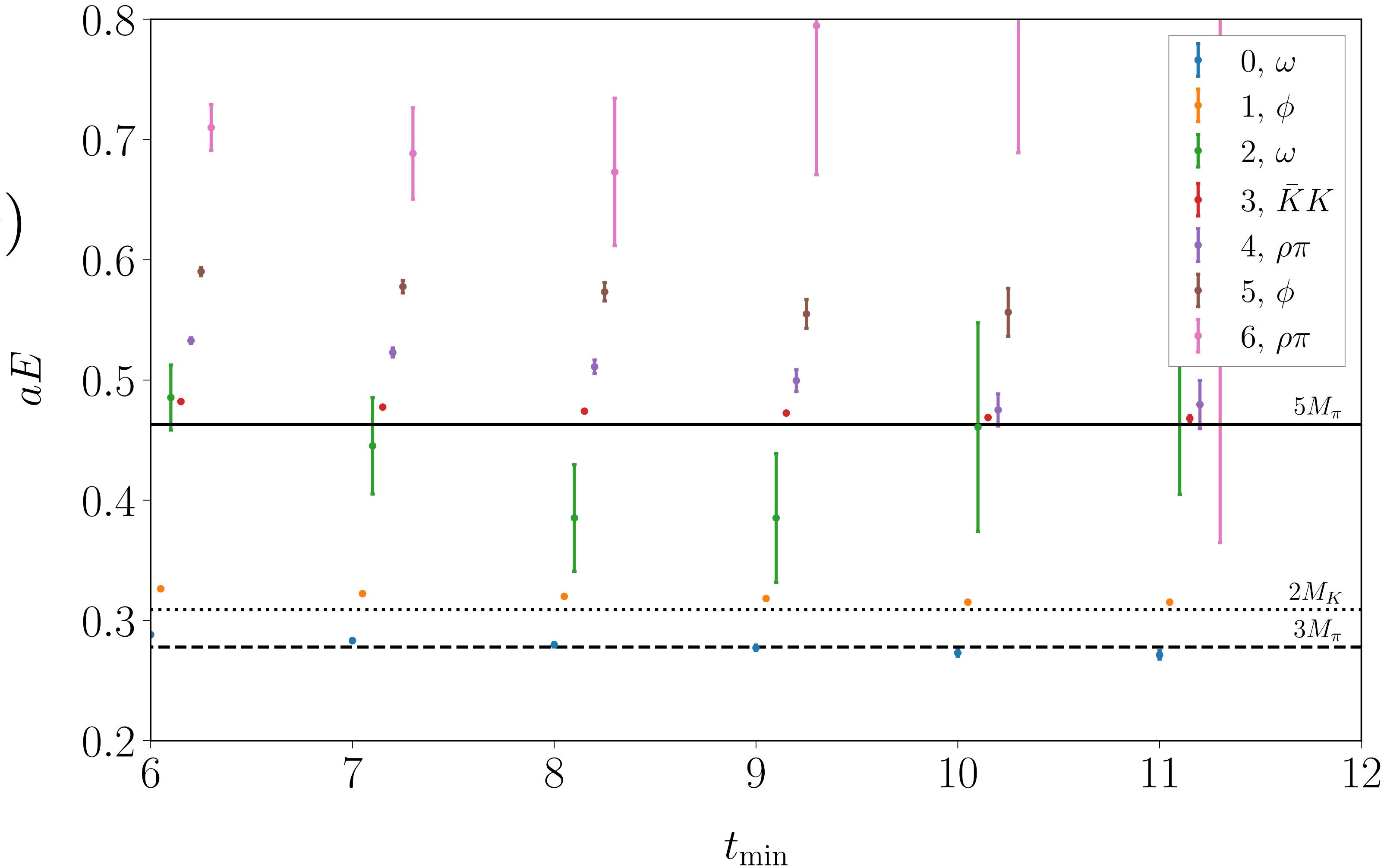
- Example: Omega at rest (I=0, T1um)

$$N_{\rm f} = 2+1,\ m_\pi = 280\text{MeV},\ 36^3 \times 128,\ N_{\rm cfg} = 350,\ N_{t_0} = 4$$

- Results: GEVP+fits (preliminary)

- Missing op:

$$\pi(0)\pi(0)\omega(0)$$



Conclusions

- Distillation continues to evolve: many interesting talks at this conference!
- Suite of code under construction for complete pipeline:

  (all public or planned for public release)

  ➔ OpPy: group theory for operator construction

  ➔ PyWick: automated Wick contractions

  ➔ QudaLaph: evaluation of tensors

  ➔ PyCorr: tensor contractions for correlators
- TODO:

  ➔ Common Subexpression Elimination: re-use subgraphs

  ➔ Three-point functions: Sparse grid sampling, or Blending

  A. Stump, J. R. Green, Phys.Rev.D 113 (2026) 3, 034513
  Z.-C. Hu, et al., 2505.01719 [hep-lat]

If you are interested in Beta testing, let us know!